

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 FEB 28 PATDPAFULL - New display fields provide for legal status
data from INPADOC
NEWS 4 FEB 28 BABS - Current-awareness alerts (SDIs) available
NEWS 5 MAR 02 GBFULL: New full-text patent database on STN
NEWS 6 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 8 MAR 22 KOREAPAT now updated monthly; patent information enhanced
NEWS 9 MAR 22 Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS 10 MAR 22 PATDPASPC - New patent database available
NEWS 11 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS 12 APR 04 EPFULL enhanced with additional patent information and new
fields
NEWS 13 APR 04 EMBASE - Database reloaded and enhanced
NEWS 14 APR 18 New CAS Information Use Policies available online
NEWS 15 APR 25 Patent searching, including current-awareness alerts (SDIs),
based on application date in CA/CAPLUS and USPATFULL/USPAT2
may be affected by a change in filing date for U.S.
applications.
NEWS 16 APR 28 Improved searching of U.S. Patent Classifications for
U.S. patent records in CA/CAPLUS
NEWS 17 MAY 23 GBFULL enhanced with patent drawing images
NEWS 18 MAY 23 REGISTRY has been enhanced with source information from
CHEMCATS
NEWS 19 JUN 06 The Analysis Edition of STN Express with Discover!
(Version 8.0 for Windows) now available
NEWS 20 JUN 13 RUSSIAPAT: New full-text patent database on STN
NEWS 21 JUN 13 FRFULL enhanced with patent drawing images
NEWS 22 JUN 27 MARPAT displays enhanced with expanded G-group definitions
and text labels
NEWS 23 JUL 01 MEDICONF removed from STN
NEWS 24 JUL 07 STN Patent Forums to be held in July 2005
NEWS 25 JUL 13 SCISEARCH reloaded

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN

07/15/2005 09927684.trn

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 12:50:10 ON 15 JUL 2005

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 12:50:21 ON 15 JUL 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 JUL 2005 HIGHEST RN 855334-87-1

DICTIONARY FILE UPDATES: 14 JUL 2005 HIGHEST RN 855334-87-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

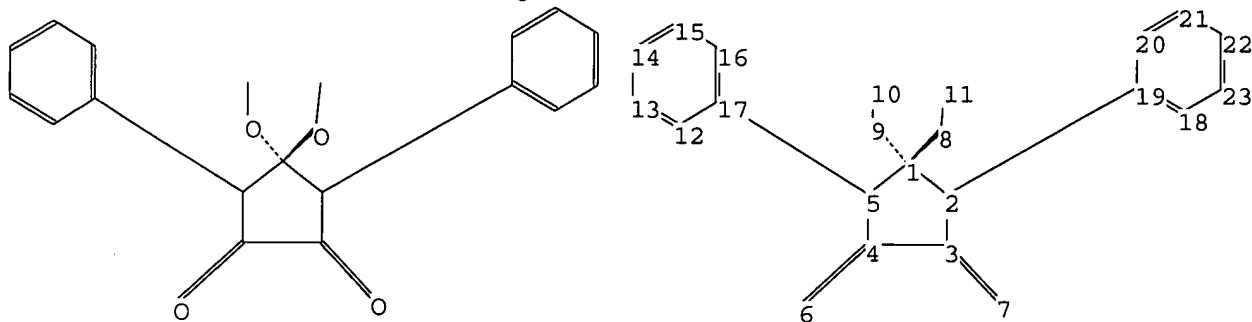
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\09927684.str



chain nodes :

6 7 8 9 10 11

ring nodes :

1 2 3 4 5 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

1-8 1-9 2-19 3-7 4-6 5-17 8-11 9-10

ring bonds :

1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23
19-20 20-21 21-22 22-23

exact/norm bonds :

1-8 1-9 3-7 4-6 8-11 9-10

exact bonds :

1-2 1-5 2-3 2-19 3-4 4-5 5-17

normalized bonds :

12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

isolated ring systems :

containing 1 : 12 : 18 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom

19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

Stereo Bonds:

8-1 (Single Wedge).

Stereo Chiral Centers:

1 (Parity=Don't Care)

07/15/2005 09927684.trn

Stereo RSS Sets:

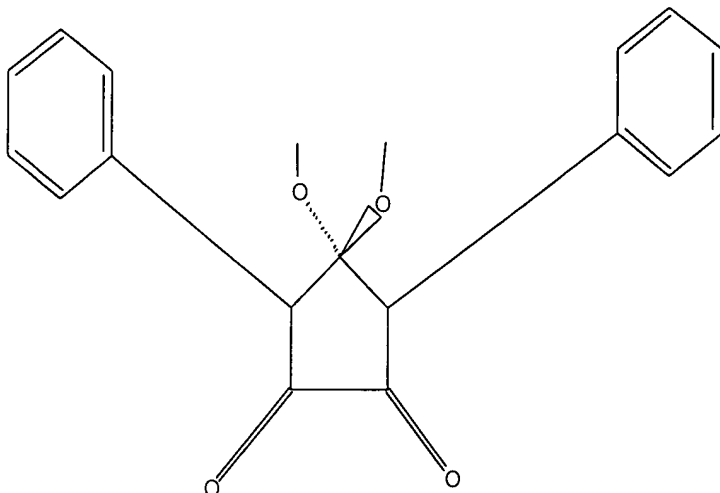
Type=Relative (Default). 1 Nodes= 1

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 12:50:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 56 TO 504
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 12:50:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 229 TO ITERATE

100.0% PROCESSED 229 ITERATIONS
SEARCH TIME: 00.00.01

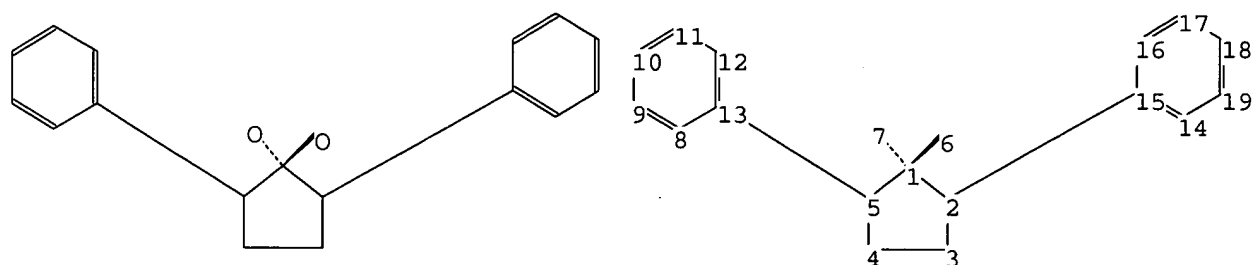
L3 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\09927684a.str

0 ANSWERS

0 ANSWERS



chain nodes :

6 7

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

1-6 1-7 2-15 5-13

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16
16-17 17-18 18-19

exact/norm bonds :

1-6 1-7

exact bonds :

1-2 1-5 2-3 2-15 3-4 4-5 5-13

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17 17-18 18-19

isolated ring systems :

containing 1 : 8 : 14 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

Stereo Bonds:

6-1 (Single Wedge).

Stereo Chiral Centers:

1 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 1

L4 STRUCTURE UPLOADED

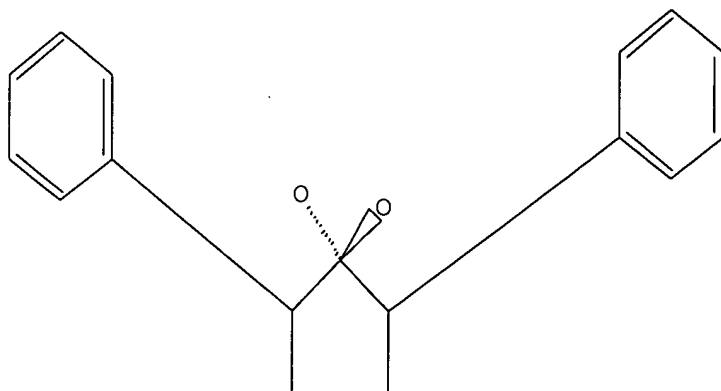
=> d 14

L4 HAS NO ANSWERS

L4 STR

07/15/2005

09927684.trn



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 12:52:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 0 TO 0

0 ANSWERS

L5 0 SEA SSS SAM L4

=> s 14 sss full

FULL SEARCH INITIATED 12:52:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 109 TO ITERATE

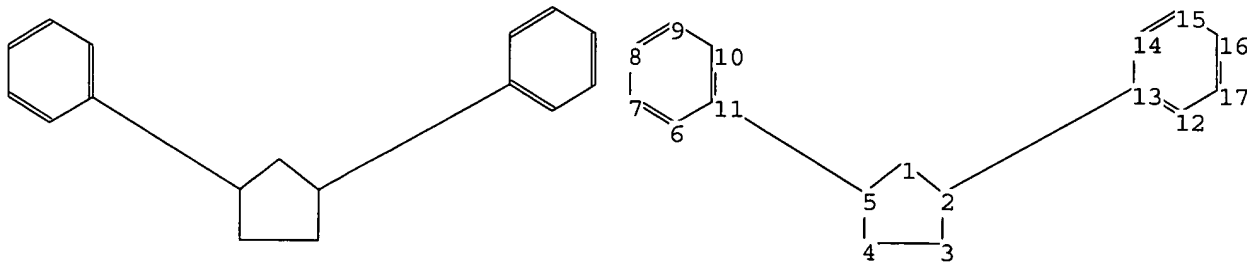
100.0% PROCESSED 109 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L6 0 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\09927684b.str



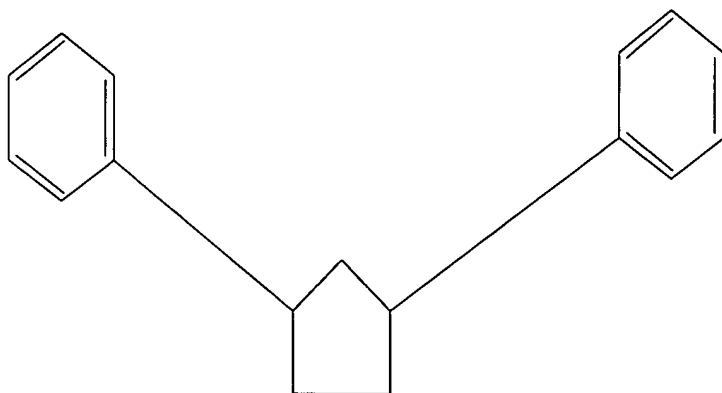
07/15/2005 09927684.trn

ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
2-13 5-11
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact bonds :
1-2 1-5 2-3 2-13 3-4 4-5 5-11
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L7 STRUCTURE UPLOADED

=> d 17
L7 HAS NO ANSWERS
L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17
SAMPLE SEARCH INITIATED 12:53:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 4323 TO ITERATE

46.3% PROCESSED 2000 ITERATIONS 12 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

07/15/2005 09927684.trn

PROJECTED ITERATIONS: 82518 TO 90402
PROJECTED ANSWERS: 213 TO 823

L8 12 SEA SSS SAM L7

=> s l7 sss full
FULL SEARCH INITIATED 12:53:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 85334 TO ITERATE

100.0% PROCESSED 85334 ITERATIONS
SEARCH TIME: 00.00.01

451 ANSWERS

L9 451 SEA SSS FUL L7

=> FIL CAPLUS
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 484.85 | 485.06 |

FILE 'CAPLUS' ENTERED AT 12:53:34 ON 15 JUL 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 15 Jul 2005 VOL 143 ISS 4
FILE LAST UPDATED: 14 Jul 2005 (20050714/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l9
L10 189 L9
=> s l10 and chromophores
16615 CHROMOPHORES
L11 0 L10 AND CHROMOPHORES

=> s l10 and chromophore
23539 CHROMOPHORE
16615 CHROMOPHORES
32936 CHROMOPHORE
(CHROMOPHORE OR CHROMOPHORES)
L12 1 L10 AND CHROMOPHORE

=> s l10 and infrared
233303 INFRARED

5 INFRAREDS
 233306 INFRARED
 (INFRARED OR INFRAREDS)
 573630 IR
 4937 IRS
 577233 IR
 (IR OR IRS)
 649309 INFRARED
 (INFRARED OR IR)

L13 13 L10 AND INFRARED

=> s l13 and py<=2000
 20650035 PY<=2000

L14 12 L13 AND PY<=2000

=> d l12 ibib abs hitstr tot

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1931:27044 CAPLUS

DOCUMENT NUMBER: 25:27044

ORIGINAL REFERENCE NO.: 25:2999c-e

TITLE: Dyes derived from oxalyldibenzyl ketone

AUTHOR(S): Saletore, S. A.; Chakravarti, Gopal Chandra

SOURCE: Proc. 15th Indian Sci. Cong. (1928) 152

DOCUMENT TYPE: Journal

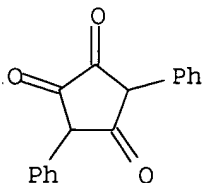
LANGUAGE: Unavailable

AB Hydroxyimidazoles obtained by condensing phenanthraquinone and acenaphthaquinone with salicylaldehyde in the presence of NH₃ are all colorless crystalline compds. (Japp and Streatfield, J. Chemical Society 41, 146(1882) and others), while those derived from substituted salicylaldehydes are colored (Sircar and Sircar, C. A. 17, 2880). It was therefore anticipated that the imidazole from oxalyldibenzyl ketone and salicylaldehyde would likewise be colorless; whereas this compound was obtained as a deep brown crystalline product with marked chromophoric properties. This is evidence in support of the observation made recently (C., C. A. 20, 207) that oxalyldibenzyl ketone is a much better **chromophore** than phenanthraquinone or acenaphthaquinone, although the latter bodies contain condensed benzene nuclei. Several other imidazoles derived from oxalyldibenzyl ketone on the one hand and vanillin, nitrosalicylaldehyde, p- and m-HOC₆H₄CHO, resorcyaldehyde, bromosalicylaldehyde, etc., on the other, are also found to be deeply colored. No details are given.

IT 7003-69-2, 1,2,4-Cyclopentanetrione, 3,5-diphenyl-
 (dyes from)

RN 7003-69-2 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



=> d l13 ibib abs hitstr tot

L13 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:148151 CAPLUS

DOCUMENT NUMBER: 138:195813

TITLE: Heat-developable photographic imaging material showing improved silver color tone for IR-laser imaging system

INVENTOR(S): Hanyu, Takeshi

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

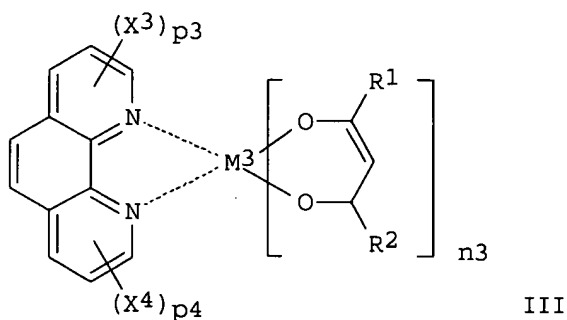
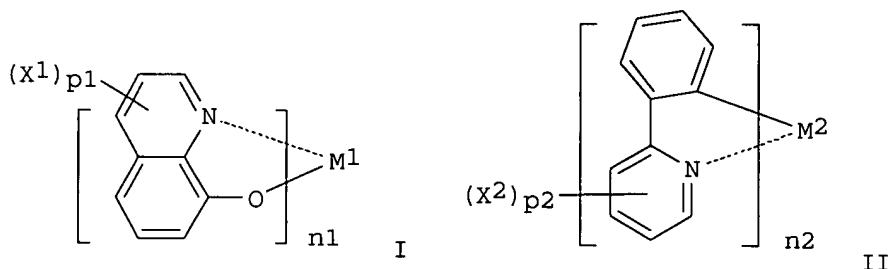
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| JP 2003057781 | A2 | 20030226 | JP 2001-246531 | 20010815 |
| PRIORITY APPLN. INFO.: | | | JP 2001-246531 | 20010815 |
| OTHER SOURCE(S): | MARPAT | 138:195813 | | |

GI



III

AB A heat-developable photog. imaging material comprises on a support photosensitive Ag halide grains, organic Ag salts, organic Ag salt-reducing agents, and binders, wherein the photog. imaging material includes at least one heterocyclic metal complex compound selected from I, II, and III (R₁, R₂, X₁₋₄ = H, halo, C₁₋₂₀-alkyl, alkenyl, alkoxy, alkylamino, alkylsulfonyl, alkylcarbonyl, alkylthio, aromatic, heterocycle; M₁₋₃ = metal atom; p₁, p₂, p₃, p₄, n₁, n₂, n₃ = 1-3). The photog. imaging material contains a specific phthalazine compound, a specific mercapto compound, and a

specific disulfide compound The photosensitive Ag halide grains have an average

particle size of 10-60 nm, are doped with Ir, Rd, and/or Ru, and are spectrally sensitized by a specific IR sensitizing dye. The reducing agent is a specific bisphenol compound and the binder is crosslinked by an isocyanate compound, a vinylsulfonyl compound, an epoxy compound, and/or an alkoxy silane compound The photog. imaging material shows improved silver color tone and scratch-resistance.

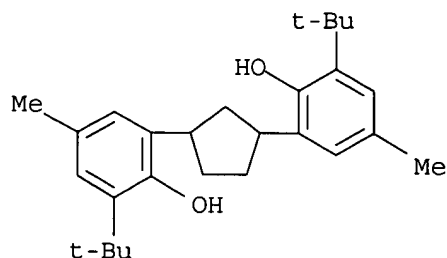
IT 498579-30-9

RL: DEV (Device component use); USES (Uses)

(organic Ag salt-reducing agent in heat-developable photog. film showing improved silver color tone)

RN 498579-30-9 CAPLUS

CN Phenol, 2,2'-(1,3-cyclopentanediy)bis[6-(1,1-dimethylethyl)-4-methyl-
(9CI) (CA INDEX NAME)



L13 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:298932 CAPLUS

DOCUMENT NUMBER: 133:223657

TITLE: Use of **infrared** dyes for transmission laser welding of plastics

AUTHOR(S): Jones, I. A.; Hilton, P. A.; Sallavanti, R.

CORPORATE SOURCE: TWI, Cambridge, UK

SOURCE: Laser Institute of America [Publication] (2000),
87(Pt. 1, Proceedings of the Laser Materials
Processing Conference, 1999), B/71-B/79
CODEN: LIAAED

PUBLISHER: Laser Institute of America

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A technique has been developed for transmission laser welding plastics with IR dye, creating a joint almost invisible to the human eye. In typical applications for laser welding of plastics, carbon black would be used as the absorbing medium for the laser energy. This new approach enables two similar clear (or colored) plastics to be joined with a minimal mark weld line. A number of dyes have been selected and assessed in terms of strength of light absorption at 1064nm wavelength with an Nd:YAG laser, as well as their visible light absorption. Lap welds have been made in clear PMMA using the IR dye mixed into Me methacrylate film as an absorbing medium at the interface between the plastic sheets. The selection of the dyes and processing methods is discussed for the new technique.

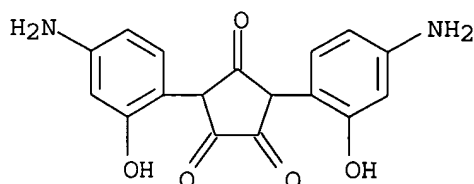
IT 291307-82-9D, derivs.

RL: MOA (Modifier or additive use); USES (Uses)

(use of IR dyes for transmission laser welding of plastics)

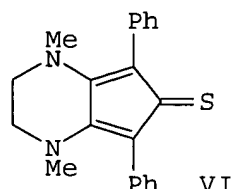
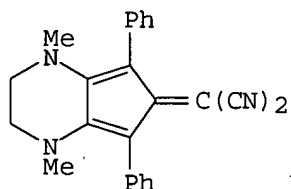
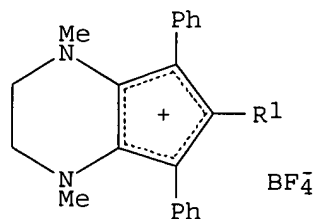
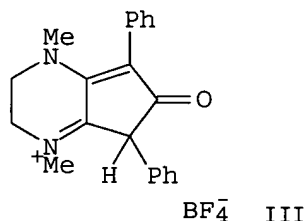
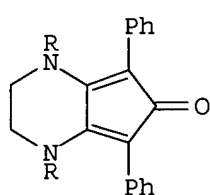
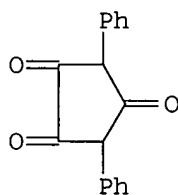
RN 291307-82-9 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3,5-bis(4-amino-2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1984:68261 CAPLUS
 DOCUMENT NUMBER: 100:68261
 TITLE: Stable cyclopentadienylium salts
 AUTHOR(S): Gompper, Rudolf; Glaeckner, Heinrich
 CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
 SOURCE: Angewandte Chemie (1984), 96(1), 48-9
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 100:68261
 GI



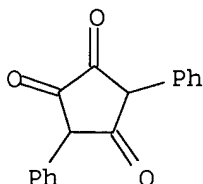
AB Reaction of diphenylcyclopentanetrione I with RNHCH₂CH₂NHR (R = Me, Ph) gave condensed cyclopentadienones II; protonation of II (R = Me) with HBF₄ occurred at a C atom to give III. Treatment of II (R = Me) with EtO⁺ BF₄⁻ gave cyclopentadienylium compound IV (R₁ = OEt), which reacted with amines to give IV (R₁ = NMe₂, pyrrolidino, morpholino). IV (R₁ = NMe₂) reacted with CH₂(CN)₂ to give fulvene V and with Na₂S to give thione VI.

IT 7003-69-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with ethylenediamine derivs.)

RN 7003-69-2 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:86799 CAPLUS

DOCUMENT NUMBER: 90:86799

TITLE: Structure of 2-benzoyl-1,3,4-triphenyl-1-cyclopentanol, reduction product of 1,3-diphenyl-2-propene-1-one

AUTHOR(S): Gaweda, Maria; Kawalek, Bozena; Lebioda, Lukasz; Mirek, Julian; Ciechanowicz-Rutkowska, Maria

CORPORATE SOURCE: Inst. Chem., Jagiellonian Univ., Krakow, Pol.

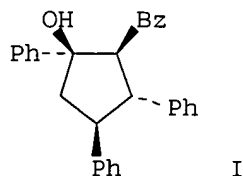
SOURCE: Polish Journal of Chemistry (1978), 52(9), 1747-51

CODEN: PJCHDQ; ISSN: 0137-5083

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



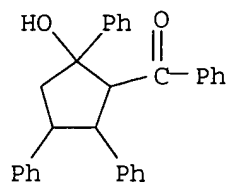
AB The Zn reduction of PhCOCH:CHPh in HOAc gave the expected monomeric products, $(\text{PhCOCH}_2\text{CHPh})_2$, and I the structure of which was determined by x-ray crystallog. The IR and mass spectra of I were related to the configuration of the substituents about the cyclopentane ring in I; H bonding between the OH and CO group was noted.

IT 33418-22-3

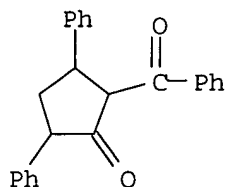
RL: RCT (Reactant); RACT (Reactant or reagent)
(crystal structure, mol. structure, and spectra of)

RN 33418-22-3 CAPLUS

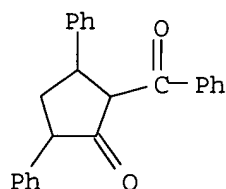
CN Methanone, (2-hydroxy-2,4,5-triphenylcyclopentyl)phenyl- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1967:453838 CAPLUS
 DOCUMENT NUMBER: 67:53838
 TITLE: Ring contraction reactions of 2,4,6-triphenyl-o-quinol acetate. Thermochromisms of substituted cyclopentadienones
 AUTHOR(S): Dimroth, Karl; Perst, Hartwig; Mueller, Karl Hans
 CORPORATE SOURCE: Univ. Marburg/Lahn, Marburg/Lahn, Fed. Rep. Ger.
 SOURCE: Chemische Berichte (1967), 100(6), 1850-7
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA Issue.
 AB Alkali treatment of 2,4,6-triphenyl-o-quinol acetate (I) in the presence of air O gave a colorless 3,5-diphenyl-2-benzoylcyclopentadienone dimer whose constitution may be 1a,3,4,6-tetraphenyl-2,7-dibenzoyl-4,7-methanoinden-8-one (II) or 1a,3,5,7-tetraphenyl-2,4-dibenzoyl-4,7-methanoinden-8-one (III). The dimer exists in temperature-dependent equilibrium with its red monomer and showed thermochromism. Under exclusion of O, I gave the corresponding completely enolized diphenyl-benzoylcyclopentenone (IV). Reactions, *ir*, and N.M.R. spectra are discussed.
 IT **15295-64-4DP**, Cyclopentanone, 2-benzoyl-3,5-diphenyl-, copper complex **15295-64-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 15295-64-4 CAPLUS
 CN Cyclopentanone, 2-benzoyl-3,5-diphenyl- (8CI) (CA INDEX NAME)



RN 15295-64-4 CAPLUS
 CN Cyclopentanone, 2-benzoyl-3,5-diphenyl- (8CI) (CA INDEX NAME)



L13 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:94760 CAPLUS

DOCUMENT NUMBER: 66:94760

TITLE: Reaction of anisole and phenetole with cyclopentanone in the presence of $\text{BF}_3 \cdot \text{H}_3\text{PO}_4$ complex

AUTHOR(S): Strashnenko, A. V.; Zavgorodnii, S. V.

CORPORATE SOURCE: Politekh. Inst., Kiev, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1967), 3(1), 91-7

CODEN: ZORKAE; ISSN: 0514-7492

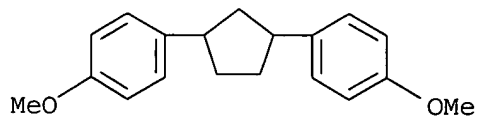
DOCUMENT TYPE: Journal

LANGUAGE: Russian

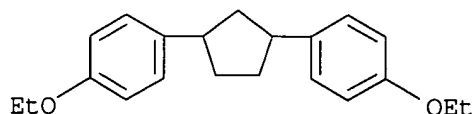
GI For diagram(s), see printed CA Issue.

AB A previously used method (CA 63, 523e) was applied in the reaction of PhOMe, PhOEt, or PhOH with cyclopentanone (I) over $\text{BF}_3 \cdot \text{H}_3\text{PO}_4$ catalyst in H_2SO_4 . E.g., with 3:1:1 mol. ratio PhOMe-I-catalyst at room temperature in 216 hrs. the following were obtained: 1,1-bis(4-methoxyphenyl)cyclopentane, 12.8%, b. 191-200°/2.5, m. 115° (MeOH); p-cyclopentylanisole, 18.9%, b. 93.5°/2, d_{20} 1.0070, n_{20D} 1.5318; 1,4-bis(4-methoxyphenyl)cyclopenta-1,3-diene (II), 14.0%, m. 232-5° (decomposition), and tar. Other reaction conditions gave different product yields. Synthesis of 1.5 g. II was also carried out by heating 9 hrs. at 60° a mixture of 10 g. Et ester of β -anisoylpropionic acid, 6.5 g. p-methoxyacetophenone, and 3.3 g. NaNH_2 in 150 ml. anhydrous C_6H_6 , and working up the reaction mixture; with 6:1:1.5 mole ratio PhOEt-I-catalyst at room temperature for 216 hrs., the following products were obtained: 1,1-bis(4-ethoxyphenyl)cyclopentane, 13.5%, m. 132-5° (MeOH); p-cyclopentylphenetole, 39.7%, b. 126°/3, d_{20} 0.9921, n_{20D} 1.5250; 1,4-bis(4-ethoxyphenyl)cyclopenta-1,3-diene (III), 18.7%, m. 201-2° (decomposition) (PhMe); and tars 0.8%. Hydrogenation of III over Raney Ni in PhMe gave 1,3-bis(4-ethoxyphenyl)cyclopentane, m. 65-5.5° (petroleum ether-MeOH), in 82.5% yield. Heating 3.8 g. III with 1.35 g. maleic anhydride in boiling PhMe 21 hrs. gave Diels-Alder addition product: 85.5% 1,4-bis(4-ethoxyphenyl) - 1,4 - endo - methylenecyclohex - 2 - ene - 5,6 - dicarboxylic acid anhydride (IV), m. 168-9° (petroleum ether- CHCl_3), which on saponification gave 1,4-bis(4-ethoxyphenyl) - 1,4 - endo - methylenecyclohex-2-ene-5,6-dicarboxylic acid, m. 121-4° (C_6H_6). Oxidation of 1 g. IV with 0.85 g. KMnO_4 in 100 ml. aqueous Me_2CO gave 0.8 g. 1,3-bis(4-ethoxyphenyl)cyclopentane-4,5-dicarboxylic acid, m. 246-9° (CHCl_3). Heating 5 g. III with 4 ml. acrylonitrile in boiling PhMe gave the Diels-Alder adduct: 51.2% 2,5-bis(4-ethoxyphenyl) - 2,5 - endo - methylene-3-cyanocyclohexene, m. 116-18° (PhMe-hexane), which was oxidized with KMnO_4 in 59% yield to 2,4-bis(4-ethoxyphenyl)cyclopentanenitrile, m. 181-3° (MeOH). Condensation of 112.8 g. PhOH with 16.8 g. I in 19.6 g. H_2SO_4 at room temperature in 16 hrs. gave, after working up, 65.8% 1,1-bis(4-hydroxyphenyl)cyclopentane, m. 157.5-58° (PhMe-n-nonane), which was also obtained in 22.2% yield together with p-cyclopentylphenol (V) (31.8%) from $\text{BF}_3 \cdot \text{H}_3\text{PO}_4 / \text{H}_2\text{SO}_4$ -catalyzed condensation. Reaction of V with $\text{ClCH}_2\text{CONH}_2$ gave

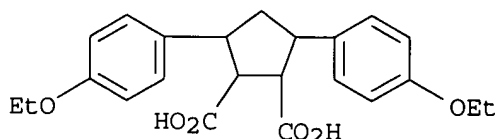
p-cyclopentylphenoxyacetamide, m. 149-50° (alc.).
IT 13693-14-6P 13693-30-6P 13693-33-9P
13693-34-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13693-14-6 CAPLUS
CN Benzene, 1,1'-(1,3-cyclopentanediy)bis[4-methoxy- (9CI) (CA INDEX NAME)



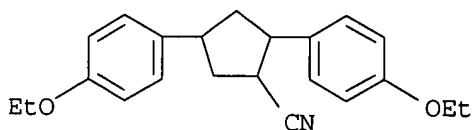
RN 13693-30-6 CAPLUS
CN Benzene, 1,1'-(1,3-cyclopentanediy)bis[4-ethoxy- (9CI) (CA INDEX NAME)



RN 13693-33-9 CAPLUS
CN 1,2-Cyclopentanedicarboxylic acid, 3,5-bis(p-ethoxyphenyl)- (8CI) (CA INDEX NAME)



RN 13693-34-0 CAPLUS
CN Cyclopentanecarbonitrile, 2,4-bis(p-ethoxyphenyl)- (8CI) (CA INDEX NAME)



L13 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:75538 CAPLUS
DOCUMENT NUMBER: 64:75538
ORIGINAL REFERENCE NO.: 64:14112g-h,14113a-g
TITLE: Diels-Alder adducts of 1,4-diphenylcyclopentadiene and maleic anhydride. Endo-exo isomerization
AUTHOR(S): Leppanen, Kaarina
CORPORATE SOURCE: Med. Fak., Univ. Helsinki
SOURCE: Ann. Acad. Sci. Fennicae, Ser. A. II (1965), No. 131, 50 pp.

DOCUMENT TYPE: Journal
 LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB The structure of 1,4-diphenyl-1,3-cyclopentadiene (I) proposed by Drake and Adams (CA 33, 62826) for the product of condensation of AcPh and BzCH₂CH₂CO₂Et was confirmed through uv, *ir*, and N.M.R. spectra; I m. 158° (C₆H₆). Reaction of I and maleic anhydride (II) in boiling C₆H₆ for 5 min. to 7 hrs. gave 1,4-diphenyl-5-norbornene-endo-cis-2,3-dicarboxylic anhydride (III), m. 154° (C₆H₆); its N.M.R. and *ir* spectra are shown. III was obtained also by treating I and II in boiling Et₂O, CHCl₃, or MePh, or by treating in CCl₄ with anhydrous AlCl₃ at room temperature; use of excess II did not influence the composition of the product. Treating 0.25 g. each of I and II 2 min. in 2.5 ml. boiling xylene (139°) gave 77.7% III, m. 145-9°. Treating 1.1 g. I and 0.54 g. II in 5 ml. boiling xylene 2.5 hrs. gave (after 2 sep. isolations) a product (in 85.3% yield) containing 64.8% endo form, which could not be purified by crystallization; reactions at 1-2.5 hrs. or use of excess II gave products with 66 ± 1.5% endo form; reactions at 30 or 45 min. gave 69.1% endo form. The endo content was determined by iodimetric titration

Heating

III alone at 160° 1.5 and 2.5 hrs. gave crystalline products, in 60 and 72% yield, resp., containing 70 ± 1.5% endo form. Heating the 1.5-hr. product with II gave a product containing 67% endo form. Hydrolysis by 100 ml. N NaOH of 3.3 g. of a 69.1% endo product from heat treatment of III, and a sep. treatment of the 2 recovered acids with Ac₂O gave, resp. (yields are before recrystn.), 1.3 g. 1,5-diphenyl-5-norbornene-endo-cis-2,3-dicarboxylic anhydride (IV), m. 142-3° (AcOH), and 0.43 g. V, the exo-cis isomer of IV, m. 165° (AcOH); the *ir* and N.M.R. spectra of IV and V are shown. The acid corresponding to IV, m. 171° (AcOEt), was recovered pure from the hydrolysis mixture, but the acid corresponding to V was obtained as a compound containing 1 mole AcOEt, m. 145-51° (AcOEt), softening at 85°. IV and V were isolated also from the product of the reaction of I and II in boiling xylene. Hydrogenation in an autoclave of an aqueous solution of the Na salt from 2 g.

III

in the presence of Raney Ni at 60-80° (finally at 120°) yielded 1.8 g. acid, m. 170-1.5°. Treating this acid with Ac₂O gave 1,4-diphenylnorbornane-endo-cis-2,3-dicarboxylic anhydride, m. 186-7° (AcOH); its *ir* spectrum is shown. From oxidation of III by alkaline KMnO₄ was isolated 1,4-diphenylcyclopentane-all-cis-1,2,3,4-tetracarboxylic acid (VI); VI.1.5H₂O m. 189-90° (decomposition); VI.0.5AcOEt m. 174° (decomposition); VI.0.5C₆H₆ m. 193-4° (decomposition); their *ir* spectra are shown. Evaporating an aqueous solution

of

VI.1.5H₂O gave VII, the monoanhydride of VI, sintering at 178.5°, m. 185° (AcOEt-ligroine 40-60°); the *ir* spectrum of VII is shown. Heating 0.5 g. VI.1.5H₂O with 10 ml. Ac₂O 3 hrs. on a water bath gave 0.4 g. VIII, the dianhydride of VI, m. 189.5-90° (AcOEt-ligroine); VIII was obtained also by treating VI or VII with AcCl; the *ir* spectrum of VIII is shown. Treating 2.5 g. Ag salt of VI 7 hrs. with 1.5 g. MeI in 50 ml. C₆H₆ on a water bath yielded 1.1 g. product, m. 160-3°, which on 2 crystns. gave a compound m. 165-6° (C₆H₆-ligroine). From the elemental composition and a general examination of the *ir* spectrum, the structure of this compound could be either IX or X. Shaking 1 g. IV in 100 ml. Me₂CO with 35 ml. 3% KMnO₄ 1 hr. at room temperature yielded 1-phenyl-endo-5-phenyl-exo-cis-5,6-dihydroxynorbornane-endo-cis-2,3-dicarboxylic acid (XI), m. 163-4° (decomposition); its *ir* spectrum is shown. Heating 0.4 g. XI with 10 ml. Ac₂O 1.5 hrs. on a water bath gave 1-phenyl-endo-5-phenyl-exo-5-

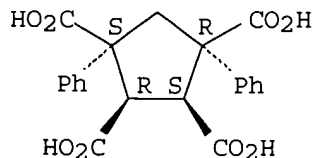
hydroxy-exo-6-acetoxynorbornane-endo-cis-2,3-dicarboxylic anhydride (XII), m. 216-17° (AcOH); its **ir** spectrum is shown. KMnO_4 oxidation of 1 g. V gave 0.40 g. 1-phenyl-endo-5-phenyl-exo-cis-5,6-dihydroxynorbornane-exo-cis-2,3-dicarboxylic acid (XIII), m. 131-3° (decomposition) ($\text{Me}_2\text{CO}-\text{C}_6\text{H}_6$); its **ir** spectrum is shown. Heating XIII with Ac_2O gave 1-phenyl-endo-5-phenyl-exo-5-hydroxy-exo-6-acetoxynorbornane-exo-cis-2,3-dicarboxylic anhydride (XIV), m. 227-8° (AcOH). Structures XI-XIV were assigned from the **ir** spectra and from analogy to results obtained elsewhere with oxidation of norbornene. It is concluded that (1) the reaction of I and II gives only the endo product III; (2) this endo adduct on heating rearranges to the exo isomer V and also a reaction occurs that leads to a new endo adduct IV; and (3) considering the work of Baldwin and Roberts (CA 58, 11179g), the concurrent processes of intramol. rearrangement and formation of the new endo product are probably two independent reactions. Mainly on these grounds, a mechanism is postulated for the isomerization of III. 97 references.

IT 5080-02-4, 1,2,3,4-Cyclopentanetetracarboxylic acid, 1,4-diphenyl-, all-cis- 5181-00-0, Ethyl acetate, compound with all-cis-1,4-diphenyl-1,2,3,4-cyclopentanetetracarboxylic acid (1:2) 5495-42-1, 1,2,3,4-Cyclopentanetetracarboxylic acid, 1,4-diphenyl-, compound with benzene (2:1) all-cis- (spectrum of)

RN 5080-02-4 CAPLUS

CN 1,2,3,4-Cyclopentanetetracarboxylic acid, 1,4-diphenyl-, all-cis- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 5181-00-0 CAPLUS

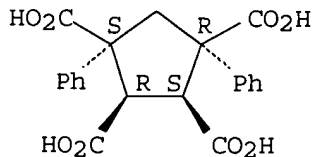
CN 1,2,3,4-Cyclopentanetetracarboxylic acid, 1,4-diphenyl-, compd. with ethyl acetate (2:1), all-cis- (8CI) (CA INDEX NAME)

CM 1

CRN 5080-02-4

CMF C21 H18 O8

Relative stereochemistry.



CM 2

07/15/2005 09927684.trn

CRN 141-78-6
CMF C4 H8 O2

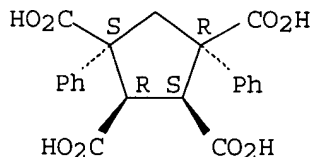
Et-O-Ac

RN 5495-42-1 CAPLUS
CN 1,2,3,4-Cyclopentanetetracarboxylic acid, 1,4-diphenyl-, compd. with
benzene (2:1), all-cis- (8CI) (CA INDEX NAME)

CM 1

CRN 5080-02-4
CMF C21 H18 O8

Relative stereochemistry.



CM 2

CRN 71-43-2
CMF C6 H6



L13 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1966:52182 CAPLUS

DOCUMENT NUMBER: 64:52182

ORIGINAL REFERENCE NO.: 64:9762f-h

TITLE: Preparation and structures of methyl
phenylpropiolate-iron carbonyl complexes. A new
dicarbonyl- π -cyclopentadienyloxy- σ -vinyliron
compound

AUTHOR(S): Dahl, Lawrence F.; Doedens, Robert J.; Hubel, Walter;
Nielsen, Jan

CORPORATE SOURCE: Univ. of Wisconsin, Madison

SOURCE: Journal of the American Chemical Society (1966),
88(3), 446-52

CODEN: JACSAT; ISSN: 0002-7863

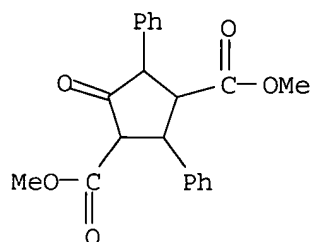
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of $\text{Fe}_2(\text{CO})_9$ with methyl phenylpropiolate has yielded four
organoiron carbonyl complexes. Three of these compds. have been
characterized on the basis of **ir** and N.M.R. spectra--two as
isomeric derivs. of tricarbonylcyclobutadieneiron and the third as

tricarbonyl-2,4-dicarbomethoxy-3,5-diphenylcyclopentadienoneiron. The fourth condensation product has required a three-dimensional single crystal x-ray investigation in order to identify it as dicarbonyl-1-carbomethoxy-2-phenyl-2- $[\pi$ -2,4-dicarbomethoxy-3,5-diphenyl-1-cyclopentadienyloxy] - σ -vinyliron. The structural features and properties of this new type complex are discussed.

IT **5576-80-7**, 1,3-Cyclopentanedicarboxylic acid, 5-oxo-2,4-diphenyl-, dimethyl ester
(preparation of)
RN 5576-80-7 CAPLUS
CN 1,3-Cyclopentanedicarboxylic acid, 5-oxo-2,4-diphenyl-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)



L13 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1966:51711 CAPLUS

DOCUMENT NUMBER: 64:51711

ORIGINAL REFERENCE NO.: 64:9619g-h

TITLE: Photoinduced reaction of azobenzene with acetyl chloride

AUTHOR(S): Lewis, G. E.; Mayfield, R. J.

CORPORATE SOURCE: Univ. Adelaide

SOURCE: Tetrahedron Letters (1966), (2), 269-71

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 64:51711

AB Irradiation of a mixture containing 50 ml. AcCl (I) and 100 mg. PhN:NPh (II) with a Hg-quartz lamp (1.5 hrs.) yielded 140 mg. N,N'-diacetyl-4-chlorohydrazobenzene (III) in 84% yield. No reaction occurred in the dark. **Ir** and N.M.R. spectra confirmed the structure for III, b0.02 132-6. Hydrolysis of the photo-induced reaction product III, followed by oxidation with NaOBr yielded 4-chloroazobenzene (IV). Reduction of pure IV with LiAlH₄, followed by exhaustive acetylation with I yielded III. An ionic mechanism is proposed for the photochem. formation of III.

IT **102959-16-0**, Cyclopentene, tetraphenyl-
(preparation of)

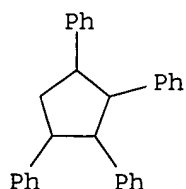
RN 102959-16-0 CAPLUS

CN Cyclopentene, tetraphenyl- (7CI) (CA INDEX NAME)

CM 1

CRN 102959-15-9

CMF C29 H26



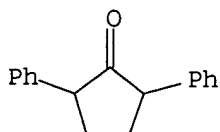
L13 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:16886 CAPLUS
DOCUMENT NUMBER: 54:16886
ORIGINAL REFERENCE NO.: 54:3359f-h
TITLE: 2,5-Diphenylcyclopentadienoneirontricarbonyl
AUTHOR(S): Schrauzer, G. N.
CORPORATE SOURCE: Monsanto Chem. Co., Dayton, O.
SOURCE: Chemistry & Industry (London, United Kingdom) (1958)
1404
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. preceding abstract The discovery of tetraphenylcyclopentadienoneirontri carbonyl led to a structural evaluation of a complex obtained by Jones, et al. (C.A. 50, 2344b), from phenylacetylene and $\text{Fe}(\text{CO})_5$ in the presence of $\text{Ni}(\text{CO})_4$ in aqueous AcOH at $60-80^\circ$. The composition of the compound was either $\text{C}_{20}\text{H}_{12}\text{O}_4\text{Fe}$ or $\text{C}_{20}\text{H}_{10}\text{O}_4\text{Fe}$. On the basis of the latter formula its structure was suggested to be that of iron tetracarbonyl bis(phenylacetylde). The extreme stability of the complex (m. $222-2.5^\circ$), however, indicated that an acetylde structure could hardly be present. Also the **infrared** spectrum revealed band of strong intensity at 1625 cm^{-1} . It was suggested that the structure of the compound was diphenylcyclopentadienoneirontricarbonyl. The chemical proof of the structure was obtained by reducing it with HI-P in AcOH . 2,5-Diphenylcyclopentanone (m. $92-94.5^\circ$) was isolated. The latter compound was identified by the method of Ruggli and Schmidlin (C.A. 40, 34088) by oxidn, with H_2CrO_4 in AcOH to yield dibenzoyl ethane.

IT 73331-36-9, Cyclopentanone, 2,5-diphenyl-
(preparation of)

RN 73331-36-9 CAPLUS

CN Cyclopentanone, 2,5-diphenyl- (6CI, 9CI) (CA INDEX NAME)



L13 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1955:28157 CAPLUS
DOCUMENT NUMBER: 49:28157
ORIGINAL REFERENCE NO.: 49:5454h-i, 5455a-g
TITLE: Ferrocene derivatives. I. The direct synthesis of substituted ferrocenes
AUTHOR(S): Pauson, P. L.

CORPORATE SOURCE: Harvard Univ.
SOURCE: Journal of the American Chemical Society (1954), 76,
2187-91
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 49:28157

AB A series of Ph-substituted ferrocenes (I) was prepared from the corresponding Ph-substituted cyclopentadienes. A mixture of cyclopentadiene (II) and phenylcyclopentadiene (III) yielded the monophenylferrocene (IV). The preparation of 1,1'-dibenzhydrylferrocene (V) from benzhydrylcyclopentadiene (VI) provided direct proof that both rings are substituted in the diacylation of ferrocene. 1,2,5-Triphenylpentane-1,5-dione (18 g.) in 500 cc. boiling glacial AcOH treated during 3 hrs. with 90 g. Zn in portions, the mixture refluxed 2 hrs., filtered hot, and poured on ice, the Zn residues extracted with a further 200 cc. hot AcOH, and the product recrystd. from cyclohexane yielded 9 g. (50%) 1,2,3-triphenylcyclopentadiene (VII), large white prisms, m. 132.5-3.5°; the mother liquors evaporated gave only an oil which was not investigated further. VII (8.2 g.) refluxed 2 hrs. with 200 cc. 95% EtOH and 20 cc. concentrated HCl, the mixture cooled, the precipitate (0.1 g.)

filtered

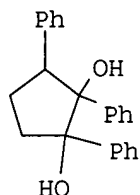
off, the filtrate heated 1 hr., concentrated to 100 cc., the addnl. precipitate (total

yield 7 g., 96%) filtered off, and the combined solid recrystd. from EtOH gave 1,2,3-triphenyl-cyclopentadiene (VIII), long, fine, pale yellow needles, m. 157-9° (sealed evacuated tube). PhLi from 35 g. PhBr and 3 g. Li in Et₂O treated at 0° with 10 g. 2-cyclopentenone, the mixture warmed to room temperature during 1 hr., stirred 1 hr. (all operations under N), poured on ice, washed with H₂O, dried, and evaporated yielded 11 g. viscous oil which crystallized partially at 0°; the crude oil distilled twice (or once with Cu bronze) was dehydrated to give 3.2 g. crude III, b. 180-220°, which was used without further purification. Crude III (0.65 g.) in Et₂O added to 10 cc. 0.5N PhLi in Et₂O, the mixture stirred 1 hr. under N, treated with 0.25 g. FeCl₃ in Et₂O, let stand overnight, and poured on ice-HCl, the Et₂O layer washed, dried, and evaporated, the residue dissolved in C₆H₆ and passed through Al₂O₃ to remove tarry impurities, and the eluate crystallized from petr. ether gave 1,1'-diphenylferrocene (IX), orange leaflets, m. 154°. MeLi from 1.4 g. Li and 14 g. MeI in 100 cc. Et₂O under N treated dropwise at room temperature with 4 g. III in 20 cc. Et₂O, 4 g. II added after 30 min., the mixture stirred another hr., cooled to 0° treated slowly with 5 g. FeCl₃, let stand overnight, and worked up in the usual manner, and the crude product chromatographed from petr. ether on Al₂O₃ (ferrocene passed through rapidly) gave IV, orange crystals, m. 109-10°; IX was held more strongly.

1,3-Diphenylcyclopentadiene (3 g.) in 50 cc. C₆H₆ added to EtMgBr from 1.5 g. EtBr and 0.32 g. Mg, the mixture refluxed 4 hrs., cooled to 0° treated with 0.7 g. FeCl₃ in Et₂O, let stand overnight, and worked up in the usual manner, and the product crystallized from MeOH gave 1,1',3,3'-tetraphenylferrocene (X), deep orange-red flat prisms, m. 220-2°. 1,2,4-Triphenylcyclopentadiene (XI) (2.5 g.) in 50 cc. C₆H₆ added to 0.012 mole BuLi in Et₂O, the mixture refluxed 2 hrs., cooled in ice, treated with 0.8 g. FeCl₃ in Et₂O, let stand overnight, and worked up, the crude product sublimed in vacuo to remove the unreacted XI, and the residue crystallized from Me₂CO gave 1,1',2,2',4,4'-hexaphenylferrocene (XII), red prisms, m. 227-8°. Diphenylfulvene reduced by the method of Sehlenk and Bergmann (C.A. 22, 4493), and the product distilled gave VI as a viscous oil which was used without further purification. VI (0.85 g.) in 10 cc. Et₂O added to 8 cc. 0.5N PhLi under N, the mixture let

stand 1 hr. at room temperature, cooled to 0°, treated with 0.2 g. FeCl₃ in 10 cc. Et₂O, let stand overnight at room temperature, poured on ice-NH₄Cl, and extracted with Et₂O, the extract washed, dried, and evaporated, the residue dissolved in cyclohexane and passed through Al₂O₃ to remove tarry impurities, the eluate evaporated, and the yellow crystalline residue, m. 161°, recrystd. from Me₂CO gave V, yellow needles, m. 162-3°. The **infrared** absorption spectra of IV, V, VIII, IX, X, XI, and XII are recorded.

IT 65102-38-7, 1,2-Cyclopentanediol, 1,2,3-triphenyl-
(preparation of)
RN 65102-38-7 CAPLUS
CN 1,2-Cyclopentanediol, 1,2,3-triphenyl- (9CI) (CA INDEX NAME)



L13 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1954:32563 CAPLUS
DOCUMENT NUMBER: 48:32563
ORIGINAL REFERENCE NO.: 48:5838b-i,5839a-i,5840a-f
TITLE: The reduction of tetracyclone
AUTHOR(S): Sonntag, N. O. V.; Linder, Seymor; Becker, Ernest I.;
Spoerri, Paul E.
CORPORATE SOURCE: Polytech. Inst. of Brooklyn, Brooklyn, NY
SOURCE: Journal of the American Chemical Society (1953), 75,
2283-92
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:32563

AB A study of the reduction of tetracyclone (tetraphenylcyclopentadienone) (I) with various reducing agents has been undertaken to find a convenient synthetic route to tetraphenylcyclopentadiene (II), which lends itself to the synthesis of fulvenes. To 1 g. I, λ_{maximum} 342 m μ (molar absorbcency index = 0.676) in C₆H₆, 262 (2.71), 335 (0.710), 512 (0.132) in cyclohexane (III), was added slowly about 2.5 Zn dust, the decolorized solution decanted while hot, cooled, and the white crystalline deposit filtered, washed with H₂O, and triturated with AcOH to leave 0.25 g. (21.7%) insol. material, evidently 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-ol (IV) AcOH solvate (V), m. 138-40° to a red liquid, reddened rapidly and lost its brilliant white fluorescence in air; the mother liquor from the solvate evaporated to dryness at room temperature in vacuo and the residue chromatographed from CCl₄ on Al₂O₃ yielded in the percolate 0.65 g. (64%) 2,3,4,5-tetraphenylcyclopentenone (VI), m. 162-3°, yellow-green in H₂SO₄, and in the iso-PrOH eluted 0.06 g. IV (total 27% based on unsolvated IV). To 1 g. I, m. 218-20°, suspended in 40 cc. AcOH was added 1.0 g. Zn dust, the curdy, gray, solid precipitate filtered off, washed successively with four 50-cc. portions of H₂O and then four 25-cc. portions of Me₂CO, and the Me₂CO washing concentrated under N in vacuo at room

temperature to give a white solid deposit, probably IV [darkened rapidly in light and air, fluoresced intensely under ultraviolet light, gave a dark red color in concentrated H₂SO₄, m. 140-8° (decomposition) with reddening at 138°]; the mother liquor from the crude V refrigerated 2 days, and the crystalline deposit filtered off, washed with 30 cc. AcOH and 50 cc. H₂O gave addnl. IV (total 0.72 g., 72%), m. 139-40° to a red liquid, darkened quickly in vacuo to a violet brown mass; careful evaporation of the 2nd mother liquor, dissoln. of the residue in CCl₄, and chromatography on Al₂O₃ gave 0.09 g. (8.9%) VI, m. 162°. 1-Methyltetraphenylcyclopentadiene-1-ol (VII), 77%, λ_{maximum} 348 (0.667) was prepared from I and MeMgI and converted with concentrated H₂SO₄ to 1,2,3,4-tetraphenylfulvene, 77%, m. 210-11°. The 1-benzyl analog (VIII) of VII, 87%, λ_{maximum} 370 (0.924), was prepared analogously and converted further to 1,2,3,4,6-pentaphenylfulvene, m. 203-4°. To 0.62 g. 2,4-(O₂N)₂C₆H₃NHNH₂ in 40 cc. dry dioxane containing 1 cc. concentrated H₂SO₄ was added 1.0 g. VI, the mixture refluxed 2 hrs. under N, cooled, poured into H₂O, the precipitate filtered off, dried in vacuo, dissolved in the min. amount of C₆H₆, chromatographed on Al₂O₃, and the lower green band eluted with C₆H₆ and evaporated to dryness, yielding 1.22 g. 2,4-dinitrophenylhydrazone of VI, red-brown solid, m. 260-1°, blue-green in H₂SO₄. VI (1.0 g.) refluxed 3 hrs. with 1.0 g. Na in 50 cc. MeOH, and the solution let stand overnight gave the Na salt of VI, colorless needles, m. 292-4°, insol. in Me₂CO, CCl₄, cold MeOH, and H₂O. V (0.30 g.) in 10 cc. AcOH containing 0.02 g. Zn dust refluxed 0.5 hr., the solution cooled, diluted with 50 cc. H₂O, and the precipitate filtered off,

washed

with Et₂O, and dried gave 0.25 g. (96%) VI, m. 160-2°. Into 5 g. I in 100 cc. AcOH and 25 g. amalgamated Zn dust was passed 10 min. dry HCl at reflux temperature and the solution quickly decanted from the residual amalgamated Zn to precipitate 4.8 g. VI, which recrystd. from EtOH, yielded 4.2 g. (84% pure VI, m. 160-2°. Into 5 g. I in 100 cc. glacial AcOH and 25 g. amalgamated Zn was passed dry HCl at reflux temperature until the color had been discharged, then 1 hr. longer, the hot liquid decanted into H₂O, and the precipitate filtered, dried, and recrystd. twice from EtOH and

once

from petr. ether (b. 90-100°) to give 0.78 g. (15.5%) 2,3,4,5-tetraphenylcyclopentanone (VIIIa), m. 175-6°, fluoresced blue-white under ultraviolet light, gave no color in concentrated H₂SO₄ [regarded previously by Dilthey, et al. (C.A. 28, 1688.9), as 2,3,4,5-tetraphenyl-3-cyclopenten-1-ol]; the mother liquors from the recrystn. of VIIIa carefully evaporated to dryness, the residue dried, dissolved in 35 cc. petr. ether, chromatographed on Al₂O₃, the lower blue-fluorescing band developed with petr. ether, eluted with C₆H₆, and the resulting 0.4 g. white waxy solid, m. 91-5° with sintering at 85°, rechromatographed from C₆H₆ on Al₂O₃ gave 0.53 g. (11%) tetraphenylcyclopentene (IX), m. 95°, λ_{maximum} 270 m μ (0.997), did not decolorize Br in CCl₄, gave no color with H₂SO₄. VIIIa (0.5 g.) added under N to PhMgBr from 1 g. Mg. and 0.5 g. PhBr in 50 cc. Et₂O, the mixture refluxed 40 min., hydrolyzed with 10% aqueous NH₄Cl, the Et₂O layer dried overnight with K₂CO₃, concentrated to 10 cc. under N in vacuo, cooled, diluted with 3 cc. 95% EtOH, and the white crystalline precipitate, m. 211-29°, recrystd. from C₆H₆ gave 0.23 g. (38%) 1,2,3,4,5-pentaphenylcyclopentanol, m. 244-6° (to a red melt), pale yellow in concentrated H₂SO₄. To 3.84 g. I suspended in 25 cc. dry C₆H₆ was added portionwise with stirring 1.34 g. AlCl₃, then after 1 hr. an addnl. 1.34 g. AlCl₃, the mixture stirred 15 hrs. at room temperature, hydrolyzed with dilute HCl, and the tan precipitate filtered off, washed with Me₂CO, and recrystd.

twice from PhMe to give 1.8 g. (46%) 1,3-diphenyl-2-oxo-1,3-dihydro-2H-

cyclopenta[1]phenanthrene (dihydrophenyclone) (X), m. 320-3°, colorless in concentrated H₂SO₄, pale orange in pyridine containing NaOEt, λ_{maximum} 280 (1.73), 291 (1.31), 335 (0.813), 303 (1.41), 351 m μ (0.853) in C₆H₆, also obtained, m. 315-18°, from phenanthrenequinone and (PhCH₂)₂CO; it had been regarded previously by Allen and VanAllan (C.A. 37, 5384.7) as VIIIa. IX (0.37 g.) in 200 cc. glacial AcOH hydrogenated 0.5 hr. at 40 lb. pressure over 0.5 g. PtO₂, the mixture filtered, the filtrate concentrated in vacuo, the residual clear oil treated with 5 cc. 95% EtOH, cooled, the resulting 0.315 g. solid chromatographed from heptane on Al₂O₃, and the lower, nonfluorescing band eluted with heptane and concentrated gave 0.31 g. tetraphenylcyclopentane (XI), pearly colorless solid, m. 154-6°, colorless in H₂SO₄, λ_{maximum} 249 (0.0733), 255 (0.0833), 260 m μ (0.0733) in III. A repetition of the Clemmensen reduction of 5 g. I but with an 8-hr. reduction time gave 2.15 g. (43%) IX, m. 95°, and 0.3 g. (6%) XI, m. 156°. I (1 g.) and 2 g. Zn dust heated 1 hr. at 270° gave 27 mg. II, m. 180°, orange in H₂SO₄, λ_{maximum} 349 m μ (1.43) in C₆H₆; 245 (2.44), 269 (2.09) 346 (1.40) in III. I (1 g.) in 60 cc. PhMe heated in a sealed tube 48 hrs. at 250-70° the dark red-violet solution cooled, concentrated in vacuo, distilled, and the red-violet, viscous residue dissolved in 10 cc. boiling Et₂O and cooled yielded 0.52 g. I, m. 219-21° (from glacial AcOH); the Et₂O mother liquor when worked up gave 0.2 g. (20%) VI; distillation of the crudely distilled solvent gave 58 cc. PhMe, b. 110-12°, and 0.5 cc. BzH, b. 178-9°, identified as 2,4-(O₂N)₂C₆H₃NHN:CHPh, m. 235-7°. I (2 g.) in 150 cc. iso-PrOH refluxed 48 hrs. was recovered quantitatively; similar results were obtained with PhMe. Absolute iso-PrOH (250 cc.), 250 cc. dry PhMe, 2.84 g. I, and 6.12 g. freshly distilled (iso-PrO)₃Al distilled slowly 2 hrs. did not give any Me₂CO; PhMe added, the mixture distilled until no more Me₂CO was detected (2 hrs.), decomposed with 85 cc. 10% H₂SO₄, the PhMe layer washed with dilute NH₄OH, then twice with H₂O, and the PhMe removed in vacuo gave a pink residue, m. 152-60°; one portion recrystd. twice from Me₂CO gave VI, colorless solid, m. 160-3°; the remainder recrystd. twice from AcOH gave VI, m. 160-2°; total yield 3.3 g. (86%). V (0.3 g.) in 10 cc. iso-PrOH and 90 cc. PhMe refluxed 2 hrs. with 0.6 g. (iso-PrO)₃Al, the mixture acidified with 8.5 cc. 10% H₂SO₄, and the PhMe layer washed with dilute NH₄OH and H₂O and evaporated to dryness in vacuo yielded 0.23 g. (88.5%) VI, m. 160-1° (from AcOH). I (1 g.) and 0.1 g. Pt black in 100 cc. refluxing AcOH under 40 lb. H pressure for 35-40 min. with shaking at 235 strokes/min., the mixture filtered, the filtrate concentrated under N in vacuo, the clear residual oil let stand, and the resulting solid recrystd. twice from 95% EtOH gave 0.46 g. (85%) XI, m. 156°, faintly blue-violet fluorescent under ultraviolet as a solid but not in solution in III. I could not be hydrogenated in AcOH, EtOAc, or C₆H₆ over 10% Pt-C or over freshly prepared Raney Ni in EtOAc or C₆H₆. II (0.2 g.) in 200 cc. AcOH hydrogenated 0.5 hr. at 40 lb. pressure over Pt black from 0.2 g. PtO₂ gave 0.18 g. (90%) XI, m. 156°. I (1 g.) refluxed 2 hrs. with 1 cc. 85% aqueous (N₂H₄).H₂O, and the clear orange solution let stand 2 days gave 40 mg. VI, m. 162°; an addnl. 0.44 g. (total yield 44%) was obtained by concentration of the mother liquor to 1/3 volume I (1.0 g.) in 50 cc. Bu₂O treated at 0-10° with 1.0 g. LiAlH₄ in 50 cc. Et₂O, and the Et₂O layer dried with MgSO₄, filtered, and concentrated under N to 1/4 volume gave 0.82 g. (81%) IV, m. 139-40°. I (2 g.) in 200 cc. dry Bu₂O added dropwise with stirring at room temperature to 2 g. LiAlH₄ in 200 cc. dry Et₂O, the mixture stirred 1 hr. at room temperature, then refluxed 2 hrs., decomposed by

the dropwise addition with cooling of 50 cc. dilute HCl (1:10), and the Et₂O layer decanted, dried with K₂CO₃, and concentrated gave VI, m. 162° (from EtOH); the mother liquor distilled, the residue taken up in C₆H₆, combined with the Et₂O filtrate, and chromatographed on Al₂O₃, and the eluate evaporated and diluted with EtOH give II, m. 180°; continued development gave 12-17% II; evaporation of the solvent and addition of EtOH yielded

1.4-1.5 g.

(75%) VI, m. 161°; a 3rd band was eluted and gave 11 mg. material, m. 231-3°, cluster of needles, not further identified. I (3.5 g.) in 20 cc. dioxane was added in 5 min. to 0.4 g. LiAlH₄ in 20 cc. dioxane, the mixture refluxed 3 hrs., hydrolyzed with 30 cc. dilute HCl (1:10),

extracted

with Et₂O, the solvents removed in vacuo, and the residue recrystd. from 50 cc. to yield 2.29 g. (65%) VI, m. 159-61°; distillation of the AcOH and chromatography of the residue in heptane on Al₂O₃ gave 7 mg. II, m. 180°. 2,4-(O₂N)₂C₆H₃NHNH₂ (1 g.) in 40 cc. purified dioxane and 2 cc. concentrated H₂SO₄ refluxed under N 2 hrs. with 1.9 g. I in 40 cc. dioxane (added during 15 min.), the mixture poured into 2 l. H₂O, the precipitated

solid

filtered off, dried, taken up in 150-200 cc. dry C₆H₆, chromatographed on Al₂O₃, and the lower red-brown band developed and concentrated under N in vacuo gave 2.54 g. (91%) 2,4-dinitrophenylhydrazones (XII) of I, violet-brown, m. 271°, blue-violet in concentrated H₂SO₄. The p-nitrophenylhydrazones of I, red-brown solid, m. 244-5°, was obtained similarly in 76% yield from 1.9 g. I and 0.76 g. p-O₂NC₆H₄NHNH₂; it gave dark blue color in concentrated H₂SO₄ and a blue-green color in alc. KOH. XII (1 g.) in alc.

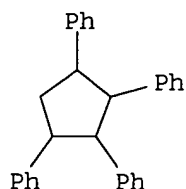
EtONa

from 1 g. Na in 40 cc. absolute EtOH heated 16 hrs. in a sealed tube at 210-20°, the white solid filtered off, the filtrate added to H₂O, the intense green suspension let stand to coagulate in the cold, and the white solid filter residue dried in vacuo, dissolved in 100 cc. C₆H₆, chromatographed on Al₂O₃, and eluted successively with C₆H₆ and CHCl₃ gave 0.237 g. 1-Et derivative (XIII) of II, m. 177-9°, orange in concentrated H₂SO₄ fluoresced under ultraviolet light; the filtrate from the coagulum extracted with Et₂O, the extract evaporated, and the residue combined with the coagulum, dissolved in 70 cc. C₆H₆, and chromatographed on Al₂O₃ with C₆H₆, CHCl₃, and iso-PrOH gave 0.025 g. XIII, m. 178-80° (total yield 40%), from C₆H₆, and 3 mg. I, m. 221. I (1 g.) and 1.0 cc. 85% aqueous N₂H₄.H₂O in 40 cc. absolute EtOH refluxed 15 min., the solution heated 16 hrs. with 1 g. Na in 30 cc. absolute EtOH in a sealed tube at 210-20°, cooled, and the precipitate recrystd. from Me₂CO yielded 0.25 g. (26%) XIII, white flakes, m. 177-9°; the initial filtrate poured into H₂O, and the light brown oily solid recrystd. twice from Me₂CO-EtOH gave 0.15 g. VI, m. 160°. The ultraviolet spectra of I, II, IV, VI, VII, VIII, VIIa, IX, 2,3,4-triphenyl-5-benzylfuran (XIV), and o-phenanthroline and the **infrared** spectra of I, IV, VI, VII, VIII, VIIa, IX, X, and XIV are reported.

IT 102959-15-9, Cyclopentane, 1,2,3,4-tetraphenyl-
155386-02-0, Cyclopentanone, 2,3,4,5-tetraphenyl-
854407-53-7, Cyclopentanol, 1,2,3,4,5-pentaphenyl-
(preparation of)

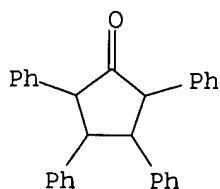
RN 102959-15-9 CAPLUS

CN Benzene, 1,1',1'',1'''-(1,2,3,4-cyclopentanetetrayl)tetrakis- (9CI) (CA INDEX NAME)



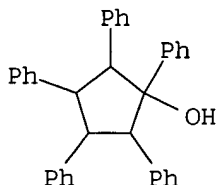
RN 155386-02-0 CAPLUS

CN Cyclopentanone, 2,3,4,5-tetraphenyl- (9CI) (CA INDEX NAME)



RN 854407-53-7 CAPLUS

CN Cyclopentanol, 1,2,3,4,5-pentaphenyl- (4CI) (CA INDEX NAME)



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ACCESSION NUMBER: 1952:66987 CAPLUS

DOCUMENT NUMBER: 46:66987

ORIGINAL REFERENCE NO.: 46:11172b-g

TITLE: Fulvenes and thermochromic ethylenes. VIII.

Infrared spectra, structure, and reactivity of the fulvenic ketones

AUTHOR(S): Bergmann, E. D.; Berthier, G.; Ginsburg, D.; Hirshberg, Y.; Lavie, D.; Pinchas, S.; Pullman, B.; Pullman, A.

CORPORATE SOURCE: Weizmann Inst. Sci., Rehovoth, Israel

SOURCE: Bulletin de la Societe Chimique de France (1951) 661-9
CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB A theor. discussion of the effects of electron distribution and induction in fulvenic ketones, particularly as relating to the mutual effects of the C:O group and induction, is given. 9-Fluorenyl- (I), 1-indenyl- (II), and 1-cyclopentadienyllithium (III) were prepared by treating the hydrocarbons in C₆H₆ with BuLi in Et₂O. I was treated with 2,3-diphenylindone (IV) for the typical preparation of 2,3-diphenyl-3-(9-fluorenyl)indanone (83% yield), m. 205-6° (from BuOH). I and tetraphenylcyclopentadienone (V) gave

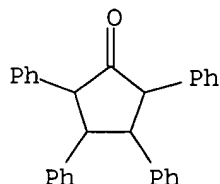
72% 2,3,4,5-tetraphenyl-3-(9-fluorenyl)-4-cyclopenten-1-one, m. 215-16° (from EtOAc). II and IV gave 57% 2,3-diphenyl-3-(1-indenyl)indanone, m. 221° (from BuOH). II and V gave 35% 2,3,4,5-tetraphenyl-3-(1-indenyl)-4-cyclopenten-1-one, m. 151° (from dilute HOAc). III and IV gave 27% 2,3-diphenyl-3-(2,4-cyclopentadienyl)-1-indanone, m. 239° (from BuOH). I and p-ClC₆H₄COCH:CHPh gave 90% 1-(p-chlorophenyl)-3-phenyl-4-biphenylene-1-butanone, m. 133° (from methylcyclohexane or PrOH). V and 2 mols. PCl₅ at 140° reacted additively to yield 2,3,4,5-tetraphenyl-2,3-dichloro-4-cyclopenten-1-one, m. 193°, with reddening (from iso-PrOH). IV in dioxane with LiAlH₄ was partially reduced to 2,3-diphenylindanone, obtained only as the dinitrophenylhydrazone, m. 125-7° (from EtOH-EtOAc). V in dioxane was reduced by LiAlH₄ to 2,3,4,5-tetraphenylcyclopentanone. 9-Fluorenone (VI) was partially reduced by LiAlH₄ to 9,9'-bifluorene, m. 243-4°, and some 9-fluorenol and fluorene. p-ClC₆H₄CH₂Cl (VII) in dioxane added to the mixture thus obtained gave some 9,9'-bis(p-chlorobenzyl)-9,9'-bifluorene (VIII), m. 220° (from BuOH), and from the mother liquors was obtained some 9-(p-chlorobenzyl)fluorene, m. 150° (from PrOH and HOAc successively). p-ClC₆H₄CH₂MgCl with VI gave 9-(p-chlorobenzyl)-9-fluorenol (IX), m. 132° (from C₆H₆ and petr. ether). IX (7 g.) refluxed 2 h. with 50 cc. AcCl and then poured on ice gave 6 g. of 9-(p-chlorobenzylidene)fluorene (X), m. 151° (from HOAc). X (1 g.) in 5 cc. dioxane and 0.2 g. LiAlH₄ in 30 cc. dioxane, refluxed 1 h., dry air passed into the solution until the red color disappeared, the solution decomposed with dilute acid, filtered, and the solid crystallized from BuOH yielded

VIII, m. 220°. I and VII were allowed to react, the product decomposed with dilute acid, and the solid filtered off and recrystd. from HOAc gave 18% white needles of 9-(p-chlorobenzyl)fluorene, m. 151°.

IT 155386-02-0, Cyclopentanone, 2,3,4,5-tetraphenyl- (preparation of)

RN 155386-02-0 CAPLUS

CN Cyclopentanone, 2,3,4,5-tetraphenyl- (9CI) (CA INDEX NAME)



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TOTAL

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SESSION

FULL ESTIMATED COST

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ENTRY

SESSION

CA SUBSCRIBER PRICE

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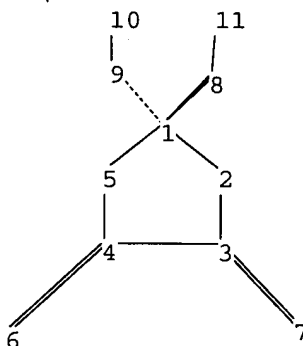
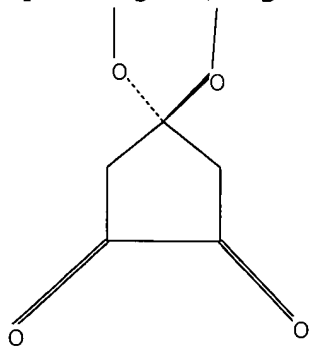
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chain nodes :

6 7 8 9 10 11

ring nodes :

1 2 3 4 5

chain bonds :

1-8 1-9 3-7 4-6 8-11 9-10

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-8 1-9 3-7 4-6 8-11 9-10

exact bonds :

1-2 1-5 2-3 3-4 4-5

07/15/2005 09927684.trn

isolated ring systems :
containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS

Stereo Bonds:

8-1 (Single Wedge).

Stereo Chiral Centers:

1 (Parity=Don't Care)

Stereo RSS Sets:

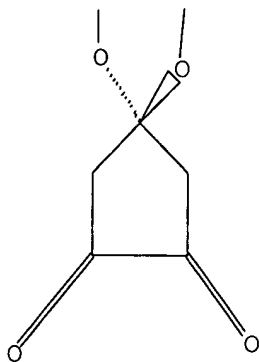
Type=Relative (Default). 1 Nodes= 1

L15 STRUCTURE UPLOADED

=> d l15

L15 HAS NO ANSWERS

L15 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l15

SAMPLE SEARCH INITIATED 12:57:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 106 TO 614

PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15

07/15/2005 09927684.trn

=> s l15 sss full

FULL SEARCH INITIATED 12:57:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 405 TO ITERATE

100.0% PROCESSED 405 ITERATIONS

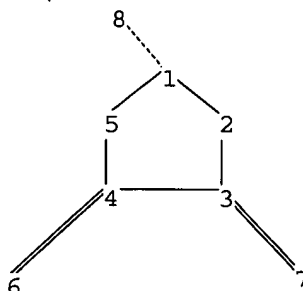
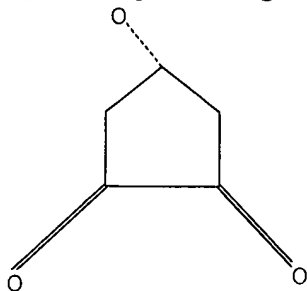
0 ANSWERS

SEARCH TIME: 00.00.01

L17 0 SEA SSS FUL L15

=>

Uploading C:\Program Files\Stnexp\Queries\09927684d.str



chain nodes :

6 7 8

ring nodes :

1 2 3 4 5

chain bonds :

1-8 3-7 4-6

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-8 3-7 4-6

exact bonds :

1-2 1-5 2-3 3-4 4-5

isolated ring systems :

containing 1 :

Match level :

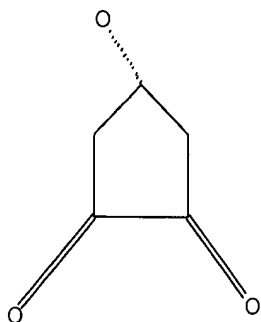
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS

L18 STRUCTURE UPLOADED

=> d l18

L18 HAS NO ANSWERS

L18 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l18
 SAMPLE SEARCH INITIATED 12:58:59 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 3278 TO ITERATE

61.0% PROCESSED 2000 ITERATIONS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 62127 TO 68993
 PROJECTED ANSWERS: 4 TO 284

L19 4 SEA SSS SAM L18

=> s l18 sss full
 FULL SEARCH INITIATED 12:59:06 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 66634 TO ITERATE

100.0% PROCESSED 66634 ITERATIONS
 SEARCH TIME: 00.00.01

294 ANSWERS

L20 294 SEA SSS FUL L18

=> FIL CAPLUS
 COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 323.95 | 887.98 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 0.00 | -10.22 |

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FILE 'CAPLUS' ENTERED AT 12:59:12 ON 15 JUL 2005
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FILE COVERS 1907 - 15 Jul 2005 VOL 143 ISS 4
FILE LAST UPDATED: 14 Jul 2005 (20050714/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 120

L21 305 L20

=> s 121 and chromophores

16615 CHROMOPHORES

L22 1 L21 AND CHROMOPHORES

=> s 121 and chromophore

23539 CHROMOPHORE

16615 CHROMOPHORES

32936 CHROMOPHORE

(CHROMOPHORE OR CHROMOPHORES)

L23 3 L21 AND CHROMOPHORE

=> s 121 and infrared

233303 INFRARED

5 INFRAREDS

233306 INFRARED

(INFRARED OR INFRAREDS)

573630 IR

4937 IRS

577233 IR

(IR OR IRS)

649309 INFRARED

(INFRARED OR IR)

L24 39 L21 AND INFRARED

=> d his

(FILE 'HOME' ENTERED AT 12:50:10 ON 15 JUL 2005)

FILE 'REGISTRY' ENTERED AT 12:50:21 ON 15 JUL 2005

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 SSS FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 0 S L4 SSS FULL

L7 STRUCTURE UPLOADED

L8 12 S L7

L9 451 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:53:34 ON 15 JUL 2005

07/15/2005 09927684.trn

L10 189 S L9
L11 0 S L10 AND CHROMOPHORES
L12 1 S L10 AND CHROMOPHORE
L13 13 S L10 AND INFRARED
L14 12 S L13 AND PY<=2000

FILE 'REGISTRY' ENTERED AT 12:56:26 ON 15 JUL 2005

L15 STRUCTURE UPLOADED
L16 0 S L15
L17 0 S L15 SSS FULL
L18 STRUCTURE UPLOADED
L19 4 S L18
L20 294 S L18 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:59:12 ON 15 JUL 2005

L21 305 S L20
L22 1 S L21 AND CHROMOPHORES
L23 3 S L21 AND CHROMOPHORE
L24 39 S L21 AND INFRARED

=> d l22 ibib abs hitstr tot

L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STM
ACCESSION NUMBER: 2003:1004592 CAPLUS
DOCUMENT NUMBER: 140:6182
TITLE: Infrared-chromophores and printing inks
containing them
INVENTOR(S): Hall, Lachlan Everett; Silverbrook, Kia
PATENT ASSIGNEE(S): Australia
SOURCE: U.S. Pat. Appl. Publ., 118 pp., Cont.-in-part of U.S.
Ser. No. 693,301.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 11
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| US 2002136972 | A1 | 20020926 | US 2001-927684 | 20010810 |
| EP 1196752 | A1 | 20020417 | EP 2000-938343 | 20000630 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 2002088064 | A1 | 20020711 | US 2001-927685 | 20010810 |
| ZA 2002000847 | A | 20030130 | ZA 2002-847 | 20020130 |
| US 2003094500 | A1 | 20030522 | US 2002-291577 | 20021112 |
| US 6843420 | B2 | 20050118 | | |
| US 2005022937 | A1 | 20050203 | US 2004-933285 | 20040903 |
| US 2005061448 | A1 | 20050324 | US 2004-949307 | 20040925 |
| US 2005064502 | A1 | 20050324 | US 2004-986403 | 20040925 |
| US 2005064503 | A1 | 20050324 | US 2004-986404 | 20040925 |
| PRIORITY APPLN. INFO.: | | | | |
| AU 1999-559 | | | | |
| AU 1999-1313 | | | | |
| AU 1999-3632 | | | | |
| AU 2000-9376 | | | | |
| AU 2000-9412 | | | | |
| AU 2000-9509 | | | | |
| AU 2000-9561 | | | | |
| AU 2000-9571 | | | | |

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| US 2000-693301 | A2 20001020 |
| AU 1999-3457 | A 19991015 |
| AU 1999-4392 | A 19991201 |
| AU 2000-5829 | A 20000224 |
| US 2000-575154 | A1 20000523 |
| WO 2000-AU775 | W 20000630 |
| US 2002-291577 | A1 20021112 |
| US 2002-322450 | A1 20021219 |

OTHER SOURCE(S): MARPAT 140:6182

AB Cycloalkane-based compds., especially IR dyes which absorb strongly in the near IR region of the spectrum but poorly in the visible regions, are disclosed. The dyes are characterized by calculated IR spectra and are suitable for use in IR-absorbing printing inks.

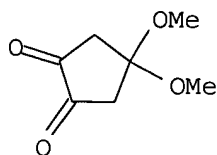
IT **603128-89-8D**, derivs.

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(dye; near-IR-absorbing **chromophores** and printing inks containing them)

RN 603128-89-8 CAPLUS

CN 1,2-Cyclopentanedione, 4,4-dimethoxy- (9CI) (CA INDEX NAME)



=> d l23 ibib abs hitstr tot

L23 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:1004592 CAPLUS

DOCUMENT NUMBER: 140:6182

TITLE: Infrared **chromophores** and printing inks containing them

INVENTOR(S): Hall, Lachlan Everett; Silverbrook, Kia
 PATENT ASSIGNEE(S): Australia

SOURCE: U.S. Pat. Appl. Publ., 118 pp., Cont.-in-part of U.S.
 Ser. No. 693,301.
 CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 11

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 2002136972 | A1 | 20020926 | US 2001-927684 | 20010810 |
| EP 1196752 | A1 | 20020417 | EP 2000-938343 | 20000630 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 2002088064 | A1 | 20020711 | US 2001-927685 | 20010810 |
| ZA 2002000847 | A | 20030130 | ZA 2002-847 | 20020130 |
| US 2003094500 | A1 | 20030522 | US 2002-291577 | 20021112 |
| US 6843420 | B2 | 20050118 | | |
| US 2005022937 | A1 | 20050203 | US 2004-933285 | 20040903 |

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|------------------------|----|----------|----------------|-------------|
| US 2005061448 | A1 | 20050324 | US 2004-949307 | 20040927 |
| US 2005064502 | A1 | 20050324 | US 2004-986403 | 20041112 |
| US 2005064503 | A1 | 20050324 | US 2004-986404 | 20041112 |
| PRIORITY APPLN. INFO.: | | | AU 1999-559 | A 19990525 |
| | | | AU 1999-1313 | A 19990630 |
| | | | AU 1999-3632 | A 19991025 |
| | | | AU 2000-9376 | A 20000814 |
| | | | AU 2000-9412 | A 20000814 |
| | | | AU 2000-9509 | A 20000818 |
| | | | AU 2000-9561 | A 20000821 |
| | | | AU 2000-9571 | A 20000821 |
| | | | US 2000-693301 | A2 20001020 |
| | | | AU 1999-3457 | A 19991015 |
| | | | AU 1999-4392 | A 19991201 |
| | | | AU 2000-5829 | A 20000224 |
| | | | US 2000-575154 | A1 20000523 |
| | | | WO 2000-AU775 | W 20000630 |
| | | | US 2002-291577 | A1 20021112 |
| | | | US 2002-322450 | A1 20021219 |

OTHER SOURCE(S): MARPAT 140:6182

AB Cycloalkane-based compds., especially IR dyes which absorb strongly in the near IR region of the spectrum but poorly in the visible regions, are disclosed. The dyes are characterized by calculated IR spectra and are suitable for use in IR-absorbing printing inks.

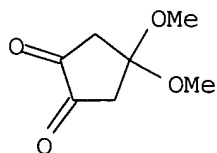
IT 603128-89-8D, derivs.

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(dye; near-IR-absorbing **chromophores** and printing inks containing them)

RN 603128-89-8 CAPLUS

CN 1,2-Cyclopentanedione, 4,4-dimethoxy- (9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:112032 CAPLUS

DOCUMENT NUMBER: 108:112032

TITLE: Synthesis of the **chromophore** of rubrolone

AUTHOR(S): Kelly, T. Ross; Echavarren, Antonio; Whiting, Andrew; Weibel, Franz R.; Miki, Yasuyoshi

CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, 02167, USA

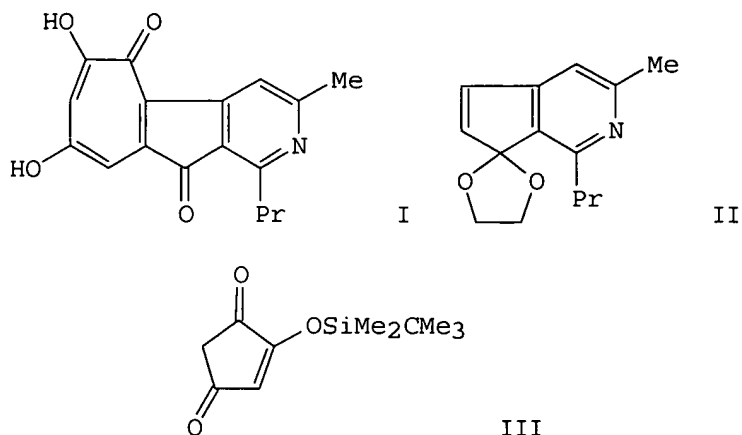
SOURCE: Tetrahedron Letters (1986), 27(50), 6049-50
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:112032

GI



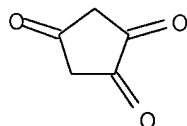
AB The **chromophore** I of rubrolone was prepared via the regiospecific cycloaddn. of the pyridanone II with the cyclopentanetrione ether III.

IT **15849-14-6**

RL: RCT (Reactant); RACT (Reactant or reagent)
(enol cyclization of)

RN 15849-14-6 CAPLUS

CN 1,2,4-Cyclopentanetrione (6CI, 8CI, 9CI) (CA INDEX NAME)



L23 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1931:27044 CAPLUS

DOCUMENT NUMBER: 25:27044

ORIGINAL REFERENCE NO.: 25:2999c-e

TITLE: Dyes derived from oxalyldibenzyl ketone

AUTHOR(S): Saletore, S. A.; Chakravarti, Gopal Chandra

SOURCE: Proc. 15th Indian Sci. Cong. (1928) 152

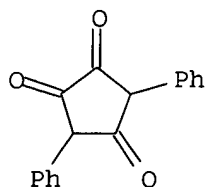
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Hydroxyimidazoles obtained by condensing phenanthraquinone and acenaphthaquinone with salicylaldehyde in the presence of NH₃ are all colorless crystalline compds. (Japp and Streatfield, J. Chemical Society 41, 146(1882) and others), while those derived from substituted salicylaldehydes are colored (Sircar and Sircar, C. A. 17, 2880). It was therefore anticipated that the imidazole from oxalyldibenzyl ketone and salicylaldehyde would likewise be colorless; whereas this compound was obtained as a deep brown crystalline product with marked chromophoric properties. This is evidence in support of the observation made recently (C., C. A. 20, 207) that oxalyldibenzyl ketone is a much better **chromophore** than phenanthraquinone or acenaphthaquinone, although the latter bodies contain condensed benzene nuclei. Several other imidazoles derived from oxalyldibenzyl ketone on the one hand and vanillin, nitrosalicylaldehyde, p- and m-HOC₆H₄CHO, resorcyaldehyde, bromosalicylaldehyde, etc., on the other, are also found to be deeply

colored. No details are given.

IT 7003-69-2, 1,2,4-Cyclopentanetrione, 3,5-diphenyl-
(dyes from)
RN 7003-69-2 CAPLUS
CN 1,2,4-Cyclopentanetrione, 3,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



=> d l24 ibib abs hitstr 1-10

L24 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:424370 CAPLUS

DOCUMENT NUMBER: 141:298526

TITLE: Bio oil from pyrolysis of cashew nut
shell-characterisation and related properties

AUTHOR(S): Das, Piyali; Sreelatha, T.; Ganesh, Anuradda

CORPORATE SOURCE: Energy Systems Engineering, Indian Institute of
Technology, Mumbai, 400076, India

SOURCE: Biomass and Bioenergy (2004), 27(3), 265-275

CODEN: BMSBEO; ISSN: 0961-9534

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Biomass in the form of cashew nut shell represents a renewable and abundant source of energy in India. Cashew nut shell (CNS) was pyrolyzed in a fixed bed pyrolysis reactor under vacuum. The CNS on heating up to 175°C produced dark brown oil (oil CO1), which was extracted, and the CNS, after the removal of oil CO1, was pyrolyzed under vacuum. The pyrolysis vapors were condensed to get a combustible oil fraction (oil CO2) as well as a noncombustible aqueous fraction. The detailed chemical compositional anal. of both the oils as well as aqueous fractions were carried out by various techniques like liquid column chromatog. 1HNMR, 13CNMR, FTIR, GC-MS. The CNS oils (CO1 and CO2) were found to be a renewable natural resource of unsatd. phenols with long linear chains and marked absence of anacardic acid. Unlike other bio oils, the CNS oils have been found to be fairly stable. The oils were completely miscible in diesel and were found to have low corrosivity towards Copper and Stainless steel, and thus promise to be a potential fuel.

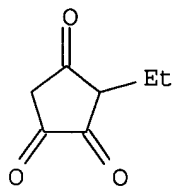
IT 4505-53-7

RL: OCU (Occurrence, unclassified); OCCU (Occurrence)

(characterization of bio oil from pyrolysis of cashew nut shell)

RN 4505-53-7 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3-ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:250308 CAPLUS

DOCUMENT NUMBER: 140:294891

TITLE: Optical filter containing near-**IR** absorbing dye and display device

INVENTOR(S): Kato, Eiichi

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 40 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

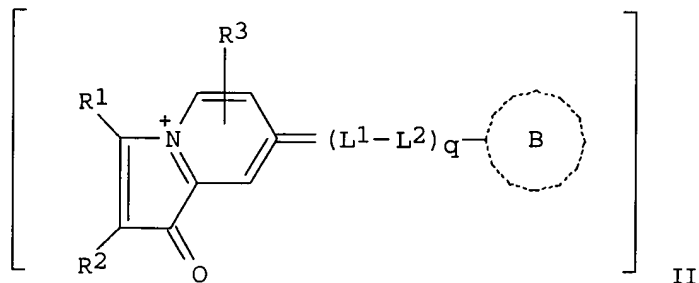
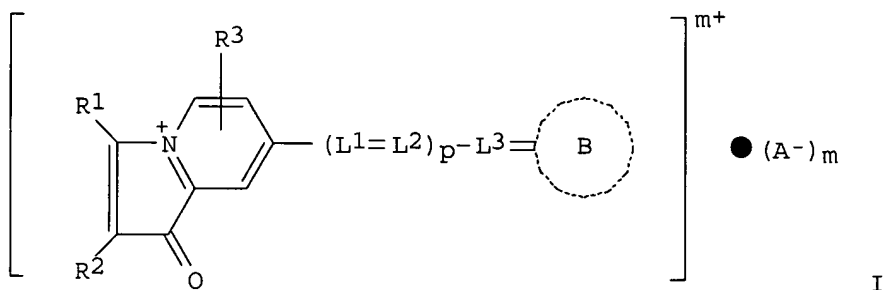
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| JP 2004093872 | A2 | 20040325 | JP 2002-254500 | 20020830 |
| PRIORITY APPLN. INFO.: | | | JP 2002-254500 | 20020830 |
| OTHER SOURCE(S): | MARPAT | 140:294891 | | |

GI



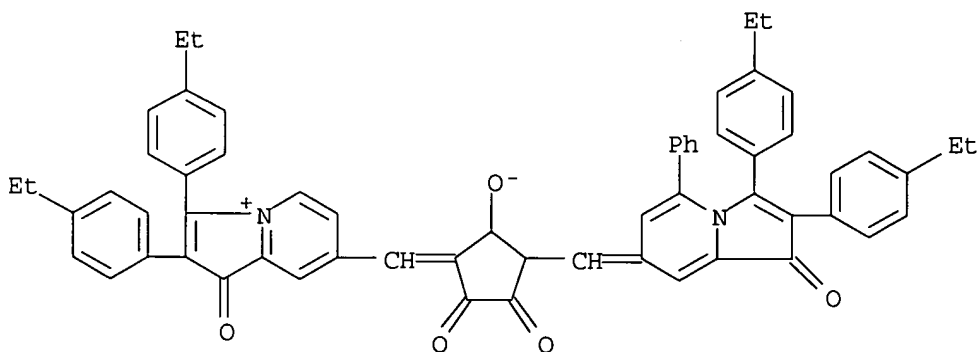
AB The optical filter comprises a filter layer on a translucent support which contains ≥ 1 near- **IR** absorbing dye selected from I (R_{1,2} = aliphatic, aryl, heterocyclyl; R₃ = H, halo, monovalent organic residue; B = organic residue forming 5- or 6-membered heterocyclyl, 5- or 6-membered condensed ring containing ≥ 1 element selected from N, O, S, Se, and Te; L₁₋₃ = methine; p = integer 1-3; q = integer 0-4; A⁻ = counter anion; and m = 1, 2) and II. The optical filter is laminated directly on the front panel of the display device such as PDP, LCD, ELD, and CRT to prevent the malfunction of a remote controller due to **IR** radiation from the screen.

IT 675819-07-5

RL: DEV (Device component use); USES (Uses)
(optical filter containing near-**IR** absorbing dye for display device)

RN 675819-07-5 CAPLUS

CN 1H-Indolizinium, 7-[[3-[[2,3-bis(4-ethylphenyl)-1-oxo-5-phenyl-7(1H)-indolizinylidene]methyl]-2-hydroxy-4,5-dioxocyclopentylidene]methyl]-2,3-bis(4-ethylphenyl)-1-oxo-, inner salt (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:1004592 CAPLUS

DOCUMENT NUMBER: 140:6182

TITLE: **Infrared** chromophores and printing inks containing them

INVENTOR(S): Hall, Lachlan Everett; Silverbrook, Kia

PATENT ASSIGNEE(S): Australia

SOURCE: U.S. Pat. Appl. Publ., 118 pp., Cont.-in-part of U.S. Ser. No. 693,301.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 11

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 2002136972 | A1 | 20020926 | US 2001-927684 | 20010810 |
| EP 1196752 | A1 | 20020417 | EP 2000-938343 | 20000630 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 2002088064 | A1 | 20020711 | US 2001-927685 | 20010810 |

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|------------------------|----|----------|----------------|-------------|
| ZA 2002000847 | A | 20030130 | ZA 2002-847 | 20020130 |
| US 2003094500 | A1 | 20030522 | US 2002-291577 | 20021112 |
| US 6843420 | B2 | 20050118 | | |
| US 2003022937 | A1 | 20050203 | US 2004-933285 | 20040903 |
| US 2005061448 | A1 | 20050324 | US 2004-949307 | 20040927 |
| US 2005064502 | A1 | 20050324 | US 2004-986403 | 20041112 |
| US 2005064503 | A1 | 20050324 | US 2004-986404 | 20041112 |
| PRIORITY APPLN. INFO.: | | | AU 1999-559 | A 19990525 |
| | | | AU 1999-1313 | A 19990630 |
| | | | AU 1999-3632 | A 19991025 |
| | | | AU 2000-9376 | A 20000814 |
| | | | AU 2000-9412 | A 20000814 |
| | | | AU 2000-9509 | A 20000818 |
| | | | AU 2000-9561 | A 20000821 |
| | | | AU 2000-9571 | A 20000821 |
| | | | US 2000-693301 | A2 20001020 |
| | | | AU 1999-3457 | A 19991015 |
| | | | AU 1999-4392 | A 19991201 |
| | | | AU 2000-5829 | A 20000224 |
| | | | US 2000-575154 | A1 20000523 |
| | | | WO 2000-AU775 | W 20000630 |
| | | | US 2002-291577 | A1 20021112 |
| | | | US 2002-322450 | A1 20021219 |

OTHER SOURCE(S): MARPAT 140:6182

AB Cycloalkane-based compds., especially **IR** dyes which absorb strongly in the near **IR** region of the spectrum but poorly in the visible regions, are disclosed. The dyes are characterized by calculated **IR** spectra and are suitable for use in **IR**-absorbing printing inks.

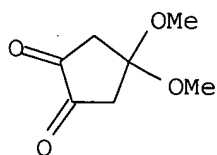
IT 603128-89-8D, derivs.

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(dye; near-**IR**-absorbing chromophores and printing inks containing them)

RN 603128-89-8 CAPLUS

CN 1,2-Cyclopentanedione, 4,4-dimethoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:853319 CAPLUS

DOCUMENT NUMBER: 139:371900

TITLE: Presensitized lithographic plates suited for computer-to-plate direct platemaking using **IR** lasers

INVENTOR(S): Kato, Eiichi; Nakamura, Ippei

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|-------------------|----------|-----------------|----------|
| JP 2003307844 | A2 | 20031031 | JP 2002-115100 | 20020417 |
| PRIORITY APPLN. INFO.: | | | JP 2002-115100 | 20020417 |
| OTHER SOURCE(S): | MARPAT 139:371900 | | | |
| GI | | | | |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The plates have, on hydrophilic supports, photoimaging layers containing **IR**-absorbing dye (i.e., photothermal converters) I and/or II [R1, R2 = aliphatic group, aryl, heterocycle; R3 = H, halo, monovalent organic group;

B = N-, O-, S-, Se-, and/or Te-containing 5-6-membered (condensed) heterocycle; L1-L3 = methine; p = 1-3 integer; q = 0-4 integer; A = counter anion; m = 0, 1]. The plates show high photosensitivity and good surface strength of image parts.

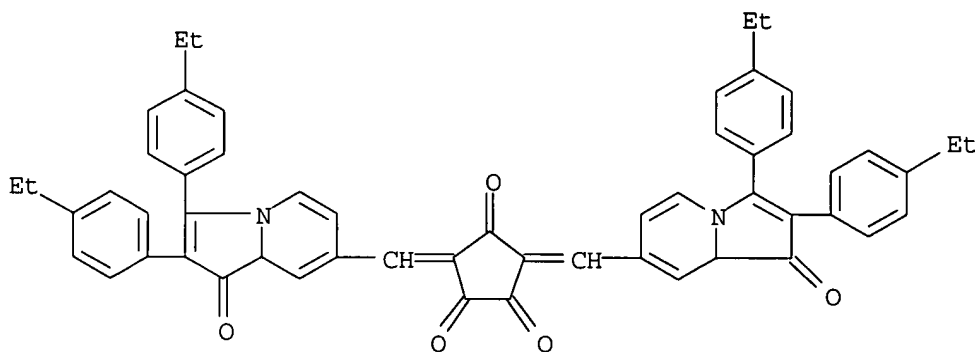
IT **620160-51-2**

RL: CAT (Catalyst use); TEM (Technical or engineered material use); USES (Uses)

(**IR**-absorbing dyes; PS plates containing oxyindolizine dyes and showing high photosensitivity and good strength of printing face)

RN 620160-51-2 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3,5-bis[[2,3-bis(4-ethylphenyl)-1,8a-dihydro-1-oxo-7-indoliziny]methylene]- (9CI) (CA INDEX NAME)



L24 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:359810 CAPLUS

DOCUMENT NUMBER: 139:133102

TITLE: Ab initio and DFT study of carbon monoxide cyclic oligomers, (CO)₂ to (CO)₆

AUTHOR(S): Sabzyan, Hassan; Noorbala, Mohammad Reza

CORPORATE SOURCE: Department of Chemistry, University of Isfahan, Esfahan, 81746-73441, Iran

SOURCE: THEOCHEM (2003), 626, 143-158

CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Structural, thermochem. stability, elec. and MO properties of (CO)_n cyclic oligomers of CO (oxocarbons) have been calculated using RHF and DFT-B3LYP levels of theory with 6-31G* basis set. Contributions of these compds. in the macroscopic properties of solid CO have been investigated. Atoms in mol. (AIM) and NBO analyses have been carried out to study in detail the nature of the C-C bonds in these mols. Population anal. has been used to search for any possible aromaticity in the rings of these cyclic oxocarbons. AIM and population anal. showed that ring bonds in the (CO)₃ mol. have an aromatic character significantly more than those in other mols. do. The results of this study showed that (CO)_n cyclic oligomers do not contribute significantly to the physicochem. properties of CO in the solid phase due to being thermodynamically instable at standard pressure and

temperature

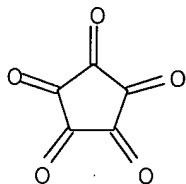
IT 3617-57-0, Cyclopentanepentone

RL: PRP (Properties)

(ab initio and DFT study on cyclic carbon monoxide oligomers)

RN 3617-57-0 CAPLUS

CN Cyclopentanepentone (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:298932 CAPLUS

DOCUMENT NUMBER: 133:223657

TITLE: Use of **infrared** dyes for transmission laser welding of plastics

AUTHOR(S): Jones, I. A.; Hilton, P. A.; Sallavanti, R.

CORPORATE SOURCE: TWI, Cambridge, UK

SOURCE: Laser Institute of America [Publication] (2000), 87(Pt. 1, Proceedings of the Laser Materials Processing Conference, 1999), B/71-B/79
CODEN: LIAAED

PUBLISHER: Laser Institute of America

DOCUMENT TYPE: Journal

LANGUAGE: English

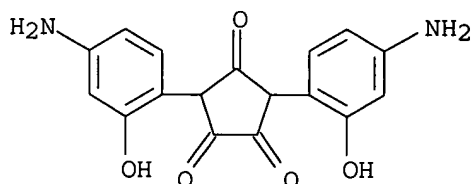
AB A technique has been developed for transmission laser welding plastics with **IR** dye, creating a joint almost invisible to the human eye. In typical applications for laser welding of plastics, carbon black would be used as the absorbing medium for the laser energy. This new approach enables two similar clear (or colored) plastics to be joined with a minimal mark weld line. A number of dyes have been selected and assessed in terms of strength of light absorption at 1064nm wavelength with an Nd:YAG laser, as well as their visible light absorption. Lap welds have been made in clear PMMA using the **IR** dye mixed into Me methacrylate film as an absorbing medium at the interface between the plastic sheets. The selection of the dyes and processing methods is discussed for the new technique.

IT 291307-82-9D, derivs.

RL: MOA (Modifier or additive use); USES (Uses)
(use of IR dyes for transmission laser welding of plastics)

RN 291307-82-9 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3,5-bis(4-amino-2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:6664 CAPLUS

DOCUMENT NUMBER: 132:165787

TITLE: Are Oxocarbon Dianions Aromatic?

AUTHOR(S): Schleyer, Paul von Rague; Najafian, Katayoun; Kiran, Boggavarapu; Jiao, Haijun

CORPORATE SOURCE: Computational Chemistry Annex, University of Georgia, Athens, GA, 30602-2525, USA

SOURCE: Journal of Organic Chemistry (2000), 65(2), 426-431
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

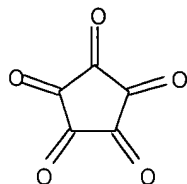
AB Assessment of the cyclic electron delocalization of the oxocarbon dianions, $C_nO_n^{2-}$ and their neutral counterparts C_nO_n ($n = 3-6$), by structural, energetic, and magnetic criteria, shows that $C_3O_3^{2-}$ is doubly aromatic (both σ and π cyclic electron delocalization), $C_4O_4^{2-}$ is moderately aromatic, but $C_5O_5^{2-}$, as well as $C_6O_6^{2-}$, are less so. Localized orbital contributions, computed by the individual gauge for localized orbitals method (IGLO), to the nucleus-independent chemical shifts (NICS) allow π effects to be dissected from the σ single bonds and other influences. The $C-C(\pi)$ contribution to $NICS(0,\pi)$ (i.e., at the center of the ring) in oxocarbon dianions decreases with ring size but shows little ring size effect at points 1.0 Å above the ring. From the same criteria, C_4O_4 exhibits cyclic electron delocalization due to partial occupancy of the σ CC bonds. However, the dissociation energies of all the neutral oxocarbons, C_nO_n , are highly exothermic.

IT 3617-57-0, Cyclopentanepentone

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(aromaticity of oxocarbon dianions)

RN 3617-57-0 CAPLUS

CN Cyclopentanepentone (7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:711657 CAPLUS

DOCUMENT NUMBER: 132:85296

TITLE: Resonance Raman investigation and semiempirical calculations of the bis(dicyanomethylene)croconate ion

AUTHOR(S): Cappa de Oliveira, L. F.; da Silva Lopes, J. G.; Barone, P. M. V. B.; Ribeiro, M. C. C.; Santos, P. S.

CORPORATE SOURCE: Instituto de Ciencias Exatas, Departamento de Quimica, Universidade Federal de Juiz de Fora, Juiz de Fora, CEP 36036-330, Brazil

SOURCE: Journal of Molecular Structure (1999), 510(1-3), 97-105

CODEN: JMOSB4; ISSN: 0022-2860

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The assignments of the optical and vibrational spectra of bis(dicyano)croconate are proposed from the resonance Raman excitation profiles as well as semi-empirical calcns. at the AM1 and PM3 levels. The absorption band at 532 nm is assigned to a $\pi \pi^*$ transition, involving a MO delocalized over the pseudo-oxocarbon ring, whereas the 1 at 442 nm is assigned to a transition localized at the CN moieties. The calcn. of the excitation profiles was performed using the transform method with a simple model of displaced harmonic oscillators, and in addition, the same model was used to reproduce the $\pi \pi^*$ absorption bandshape within the time-dependent formalism.

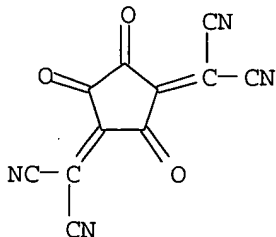
IT 75654-92-1

RL: PRP (Properties)

(resonance Raman investigation and semiempirical calcns. of (dicyanomethylene)croconate ion)

RN 75654-92-1 CAPLUS

CN Propanedinitrile, 2,2'-(2,4,5-trioxo-1,3-cyclopentanediyldiene)bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:222967 CAPLUS

DOCUMENT NUMBER: 124:342468

TITLE: The intermediates in the low-temperature photolysis of bis(diazo)cyclohexatetraone in an argon matrix

AUTHOR(S): Ohana, Tsuguyori; Yabe, Akira

CORPORATE SOURCE: National Institute Materials Chemical Research, Tsukuba, 305, Japan

SOURCE: Chemistry Letters (1996), (4), 325-6

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The photolysis of bis(diazo)cyclohexatetraone (1) was investigated in an argon matrix at 17 K. Two intermediates were formed by a consecutive decomposition of two diazo groups of 1, which were identified by UV-vis and IR spectra.

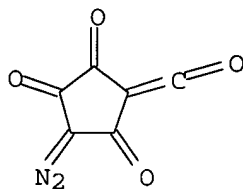
IT 176910-87-5

RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(intermediate; intermediates in the low-temperature photolysis of bis(diazo)cyclohexatetraone in an argon matrix)

RN 176910-87-5 CAPLUS

CN 1,2,4-Cyclopentanetrione, 3-carbonyl-5-diazo- (9CI) (CA INDEX NAME)



L24 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:214297 CAPLUS

DOCUMENT NUMBER: 124:300793

TITLE: Electrochemical behavior of oxocarbons on single crystal platinum electrodes. Part 3. Croconic acid oxidation on Pt(111) surfaces in acid medium

AUTHOR(S): Carbo, R.; Albalat, R.; Claret, J.; Orts, J. M.; Rodes, A.; Perez, J. M.

CORPORATE SOURCE: Departament de Química Física, Universitat de Barcelona, Martí i Franques 1, Barcelona, 08028, Spain

SOURCE: Journal of Electroanalytical Chemistry (1996), 404(1), 161-9

CODEN: JECHES; ISSN: 0368-1874

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electrochem. behavior of croconic acid (CRA) on Pt(111) electrodes was studied in acid medium by cyclic voltammetry. Its oxidation proceeds via a dual path mechanism. The direct oxidation path takes place at potentials >0.9 V, probably involving incipient surface oxide formation. The

formation of strongly adsorbed species upon CRA adsorption is influenced by the concentration of CRA and the adsorption potential. At open circuit, only

COads is formed, while at controlled potentials <0.40 V, other adsorbates, probably with more than one carbon atom, exist. These are oxidized to CO in the range 0.4-0.6 V. The activity for poison formation at open circuit is much lower for concns. >1 mM. FTIR expts. clearly indicate that carbon monoxide is not formed at potentials <0.40 V. Linearly- and bridge-bonded CO adspecies appear at potentials >0.40 V, which are oxidized to CO₂ before the direct oxidation of CRA begins. A band at 1780 cm⁻¹ indicates leuconic acid at potentials between 0.95 and 1.22 V as a product of the latter process. At higher potentials, CRA is completely oxidized to CO₂.

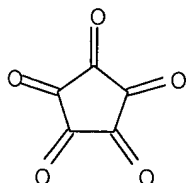
IT 3617-57-0, Leuconic acid

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation in electrochem. oxidation of croconic acid on platinum in acid solution)

RN 3617-57-0 CAPLUS

CN Cyclopentanepentone (7CI, 8CI, 9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 77.08 | 965.06 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -10.22 | -20.44 |

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